Politecnico di Torino

Engineering & Management
A.a. 2021/2025
Graduation Session July 2025

Optimization for a polymer reactor in Petrochemical Industry

Supervisor:
Arianna Alfieri
Erica Pastore
Claudio Castiglione
Daniel De Oliveira Mota

Candidate:
Alexandre Liu Guo

Abstract

The petrochemical industry plays a crucial role in the global economy, providing versatile products such as resins used in a wide range of quotidian applications. However, the complexity of multi-grade continuous production systems often results in significant operational inefficiencies, particularly in the form of "off-spec" or "non-prime" products during transitions between resin grades. This thesis addresses the challenge of optimizing sequencing and production planning for a polymer reactor within a second-generation petrochemical facility. A mixed-integer linear programming (MILP) model, introduced by the work of Abdullah, Shamayleh and Ndiaye, is implemented to minimize production and transition costs while satisfying customer demands. Real-world data from a leading Latin American petrochemical company are used to validate the model. The results demonstrate the model's ability to reduce the number of transitions and associated costs compared to current practices. The study highlights the potential of mathematical modeling as a decision-support tool for improving efficiency and aligning production with market requirements in the petrochemical sector.

Keywords: petrochemical industry, production scheduling, Mixed-Integer Linear Programming, polymer reactor, off-spec minimization, lot-sizing, optimization.

Acknowledgements

I would like to thank my entire family, who have always supported and stood by me. Especially my mother and father, who have helped me unconditionally at every step to reach my goals. I am also grateful to my brother and sister, who are my role models both as person and as professional. And to my extended family, who have cared for me and shaped the person I am today.

To my friends and classmates at Escola Politécnica, with whom I shared challenges, learning experiences, and joyful moments. Especially Beatriz, Gabriela, Pedro, and Victor.

To my friends and colleagues at Politecnico di Torino, who welcomed me and made me feel at home during my three-year exchange program in Italy.

To Escola Politécnica and the Department of Production Engineering, which provided me with academic knowledge and countless opportunities.

Finally, to Professor Dra. Arianna Alfieri who welcomed me as her advisee, guided me, and taught me through these past years for this project. I am deeply grateful for this opportunity and her mentorship.

Table of Contents

List of Tables

List of Figures

Chapter 1

Introduction

The oil industry is among the fastest-growing sectors in the world, and its relevance is strategic for the global economy. This fact is evidenced by the global revenue ranking, with three of the seven largest companies in the world being oil companies: Saudi Aramco in fourth place, Sinopec Group in fifth, and China National Petroleum in sixth place [1]. Petroleum-derived products are also ubiquitous in everyday human life, from fuels for transportation, fibers for clothing, cosmetics for beauty, packaging for products, and even various plastic utensils.

The oil industry's production chain is extensive and involves a variety of activities ranging from the exploration and production of oil fields to the commercialization of petroleum derivatives. These activities are further subdivided and often operated and executed by different companies throughout the production process. In general, the oil industry can be divided into two main sectors: Extraction & Production and the Petrochemical Industry. In the extraction phase, activities include the production of raw materials such as naphtha and natural gas liquids. On the other hand, the petrochemical sector can be further divided into 1st-generation, 2nd-generation, and 3rd-generation industries, which are respectively responsible for chemical cracking, resin polymerization, and plastic conversion. The end of the production chain involves the distribution and commercialization of final products, such as plastics in various forms, to the end consumer. In a succinct and simplified manner, the Figure 1.1 represents the production chain of the aforementioned industry.

In the current context, the petrochemical sector has become increasingly competitive due to globalization and the recent rise in demand [2]. On one hand, the industry faces commercial pressure from the World Trade Organization (WTO), and on the other hand, companies are under ecological pressure from growing environmental regulations. As a result, the scenario has become increasingly complex, challenging factories to maximize their efficiency and effectiveness to the fullest extent [3]. To achieve this goal, the sector has sought to invest in the most

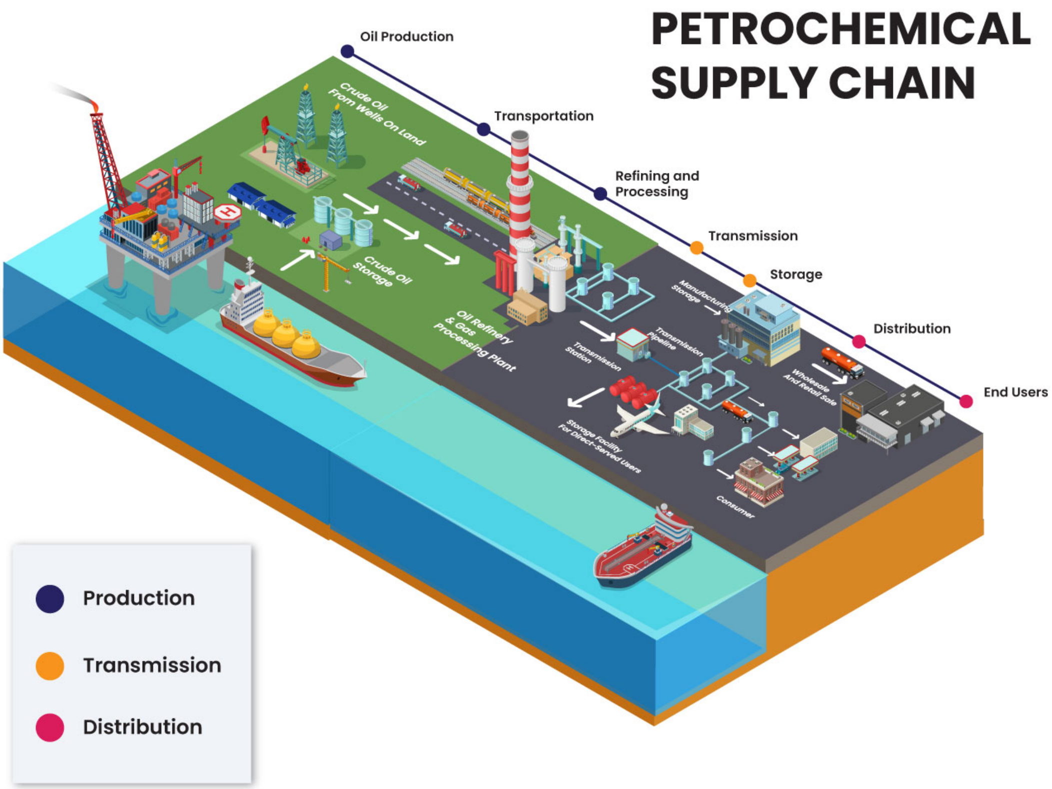

Figure 1.1: Supply chain of the petrochemical industry

modern and sophisticated tools to increase profit while simultaneously reducing costs. Examples of some instruments currently being implemented in the market include the use of Enterprise Resource Planning (ERP), supply chain management systems [4], optimization tools using linear programming [5], integer programming, heuristic or metaheuristic methods, among others.

1.1 Company's description

The company in question is a global corporation founded in 2002 through the integration of six companies, and it is currently the leading producer of thermoplastic resins (Polyethylene + Polypropylene + Polyvinyl chloride) in the Americas and the sixth largest petrochemical company in the world. Nationally, it is the only petrochemical company that integrates both the first and second generations of thermoplastic resins, playing a crucial role for third-generation industries, which are responsible for the transformation of plastics.

The full scale of the company is also reflected in its corporate status. It has over 8,000 employees across 11 countries, supporting a production capacity of more than 10 million tons of chemicals sold to 71 countries across all 5 inhabited continents, generating net revenue of over 19 billion U.S. dollars in a fiscal year. Another noteworthy point is the company's encouragement of innovative thinking. The organization is constantly seeking smart and unique solutions for its clients in order to boost their business performance while also being mindful of social and environmental impacts through its global sustainable development strategy.

1.2 Problem's scope

The present work focuses on production scheduling for the company previously described, specifically at the production unit located in the city of Mauá, São Paulo. The selection of this study was requested by a manager from the company itself, with the goal of understanding, improving, optimizing, and deepening the existing process within the organization. Additionally, it also aims to bring the academic research approach — and all of its strengths — into the institution, which is continuously seeking innovation.

The specific scope of this problem lies within the company's 2nd-generation petrochemical industry, more precisely in the polymerization process and resin production. At this stage of the production chain, these raw materials are initially directed to reactors, where they receive additives and catalysts as illustrated in the Figure 1.3. Through precise control of temperature and pressure, different types of resins are produced, each following a specific production configuration. In other words, the applied conditions determine the physical and chemical properties of the final products, resulting in a wide variety of resins [6]. This is also reflected in very diversified market demands, as each type of resin has specific properties to meet the distinct needs and applications of consumers as demonstrated in the Figures 1.5 and 1.6

In this context, it is important to introduce the term "resin grades" to differentiate the various resulting products, both for commercial purposes and academic understanding. "Grades" are subclassifications of resins that describe them as a unique material without ambiguity or further subdivisions. Within this concept, they can be grouped into "prime grades" — often referred to simply as "grades" — and "off-grades", "off-spec", or also known as "non-prime grades" in various literature sources. In the first case, the products have specific technical specifications such as density (ρ), melt flow index (MFI), viscosity, tensile strength, etc., resulting in a consistent quality and predictable material performance. As a result, the market perceives them as having higher added value and assigns them a higher monetary

Figure 1.2: Example of resin in bulk

worth. On the other hand, "off-grades" are those that do not meet any of the specific technical specifications of prime grades, making it impossible to classify these resulting resins under any established grade. Usually, they present a mix of properties which are not suitable for any specific use. Consequently, they exhibit variable characteristics and are perceived by the market as having lower added value.

That said, it is worth noting that the generation of "off-grades" during manufacturing is inevitable, since switching production from one "grade" to another requires adjustments to reactor conditions, changes in catalysts and additives, as well as possible equipment cleaning, evidenced by Figure 1.4. During this continuous procedure, there is a high probability that some of the transitions will produce this "off-grade" byproduct, which has lower commercial value [7].

The amount generated depends on the specific transition between the two "grades" [6], and therefore, companies often carry out gradual sequencing — either in ascending or descending order — in order to reduce the creation of this byproduct [8].

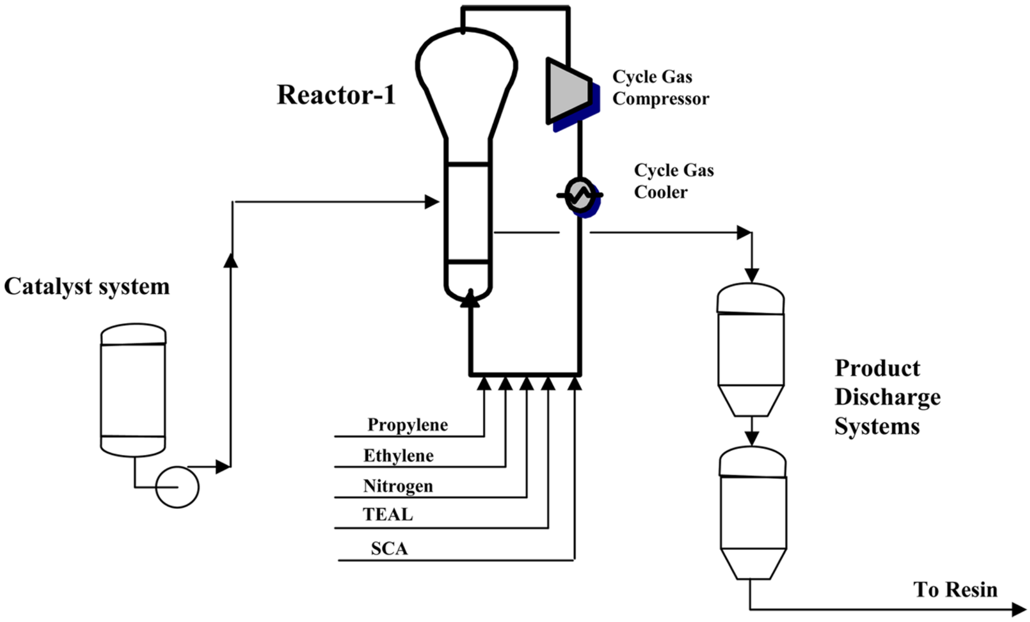

Figure 1.3: Schematic flow diagram of a resin plant

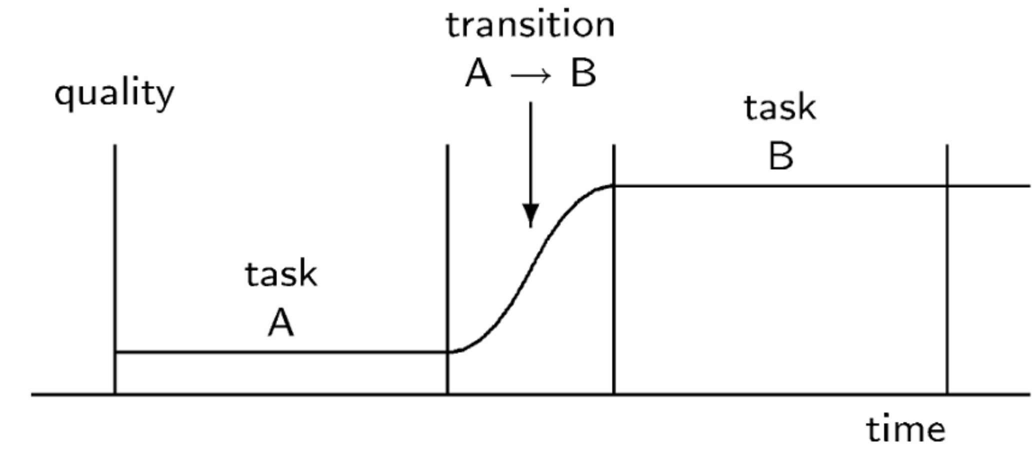

Figure 1.4: Multi-grade production process with transition

1.3 Thesis outline

Thus, the objective of this project is to optimize the manufacturing of resin "grades" by minimizing production costs and, consequently, maximizing financial returns. To achieve this, the study evaluates the company's operational production stability alongside various sequencing options and scenarios that best align with commercial demands and customer satisfaction. For a more comprehensive understanding of the overall process, two types of errors are considered: (1) Execution error – the deviation between the executed process and the scheduling plan due to variations in process parameters such as temperature, pressure, or raw material characteristics; and (2) Planning error – the deviation between the executed process and the optimal scheduling plan resulting from sequence execution decisions.

This thesis explores optimization within the petrochemical industry. It begins with an extensive literature review to deepen the understanding of the topic, followed by an examination of the current state of the art and a survey of relevant mathematical models. A suitable model is then selected to effectively address the scheduling problem. The proposed solution approach is subsequently tested using real-world instances from a specific company. Based on the analysis of the results, the thesis offers insights and proposes potential modifications to improve the current production planning practices of this business unit.

Figure 1.5: Example of resin's application in everyday

Figure 1.6: Example of final consumer good made by resins

1.4 Structure

This work is structured into five chapters: Introduction, Literature Review, Mathematical Modeling, Model Implementation and Results, and Conclusion.

Chapter 1 introduces the petrochemical industry, presents the motivation for this research, and defines the scope of the problem.

Chapter 2 provides the theoretical foundation necessary for a deeper understanding of the topic, along with a review of the state of the art based on relevant academic literature. It contextualizes the production sequencing problem within the petrochemical industry and examines methodologies, models, and strategies previously proposed or applied in similar scenarios. This establishes the conceptual and methodological groundwork for the present study.

Chapter 3 details the selected mathematical model, beginning with the underlying premises and hypotheses, followed by the objective function and the constraints of the formulation.

Chapter 4 presents the input data derived from company-specific information. The results of the test instance are then analyzed and compared with current production planning practices, offering insights into potential improvements.

Finally, Chapter 5 concludes the thesis with a summary of the main findings, a critical evaluation of the implemented model, and suggestions for future research to further refine the approach.

Chapter 2

Literature review

The literature review was conducted using the snowballing method [9]. That is, starting with the investigation of the article by Alfares [5], the understanding of the subject was expanded, complemented, and deepened through readings cited in that article, as well as other materials considered relevant to the topic. In general, the keywords that guided this search process were "petrochemical", "continuous production", "multi-grade", "off-spec", "scheduling" and among others.

This chapter aims to present the theoretical foundation and background necessary for the development of the present work. Therefore, it is essential to understand the academic context in which the study is situated, its connection to the research topic, and, finally, the proposed resolution method. To that end, key concepts from the literature will be presented, focusing mainly on mathematical modeling and production planning.

The first section provides an overview of optimization and mathematical modeling, the quantitative methodology employed in this thesis. It then introduces the concept of production planning, which is subsequently examined in greater depth through the topics of scheduling and lot-sizing. Each topic is explored in terms of its specific characteristics and associated challenges. The discussion on scheduling focuses primarily on single-machine systems involving a fixed set of products and deterministic demand. In contrast, the lot-sizing discussion emphasizes the capacitated lot-sizing problem, with particular attention to the single-level modality. A reference model for this class is presented, serving as the foundation for the final solution approach developed in this study.

2.1 Optimization and mathematical modeling

Optimization problems are characterized by complexities such as constraints and trade-offs, where one must make decisions in order to achieve the best possible outcome. Although common sense may often seem sufficient to solve such problems, an approach based on more systematic and quantitative resolution methods can indeed have a significant positive impact on system performance [10]. With that in mind, mathematical models are introduced for optimization problems, using algebraic tools for their solution. These models are defined as representations of reality, aiming to provide insights into the original problem. Therefore, when dealing with problems of this nature, certain simplifications and assumptions are made in order to determine, as accurately as possible, the likely consequences of the actions to be taken.

2.1.1 Mixed-Integer Linear Programming algorithm

Although the pursuit of optimal decision-making through analytical and quantitative approaches predates it, the term operations research as we know it today was coined during World War II. The term was used when British military officers asked scientists and engineers to analyze operational problems within the military context, such as convoy management, anti-submarine missions, and others [11].

Within this field of research, several branches emerged over time in terms of solution methods, with one of the most prominent being linear programming. This type of programming is defined as an optimization method for systems that can be represented by linear equations [12], and it marked its breakthrough in 1947, shortly after World War II, rapidly spreading alongside the expansion of computational power. This solution technique can be seen as part of a major developmental revolution, giving humanity the ability to define objectives and outline a decision path to achieve the “best” outcome when facing highly complex situations. Today, its application extends across sectors such as agribusiness, finance, education, logistics, and beyond [13].

Within the scope of the petrochemical industry, although there are several other tools available, mathematical programming models such as Mixed Integer Linear Programming (MILP) are among the most popular methods for petrochemical production and inventory planning [14]. An MILP model is a type of linear programming in which the objective function and constraints are linear, but with the particularity that some or all of the variables are restricted to integer values [15].

2.2 Production planning

Production planning in companies is generally carried out in a segregated manner, both hierarchically and functionally. The process is sequential, where top-level decisions shape and constrain the subsequent ones. In this approach, the time horizon decreases along the decision-making chain, while the level of detail increases.

Additionally, there is a reverse flow of information in which lower levels report their adherence back to higher levels for evaluation and monitoring purposes. However, it becomes evident that this procedure is suboptimal in its design, as it lacks a systemic and holistic perspective [16].

According to Gelders and Wassenhove [16], the hierarchies typically present in companies can be classified as high level, mid level, and low level. At the high level, decisions are made based on aggregated information, primarily to determine the quantity and timing of product production. These decisions are then broken down at the mid level, where the quantity and timing of production are again established, but this time for the product components. Finally, at the low level, based on the previous information, short-term scheduling is defined, and specific resources are allocated. An information flow diagram is exemplified in the Figure 2.1.

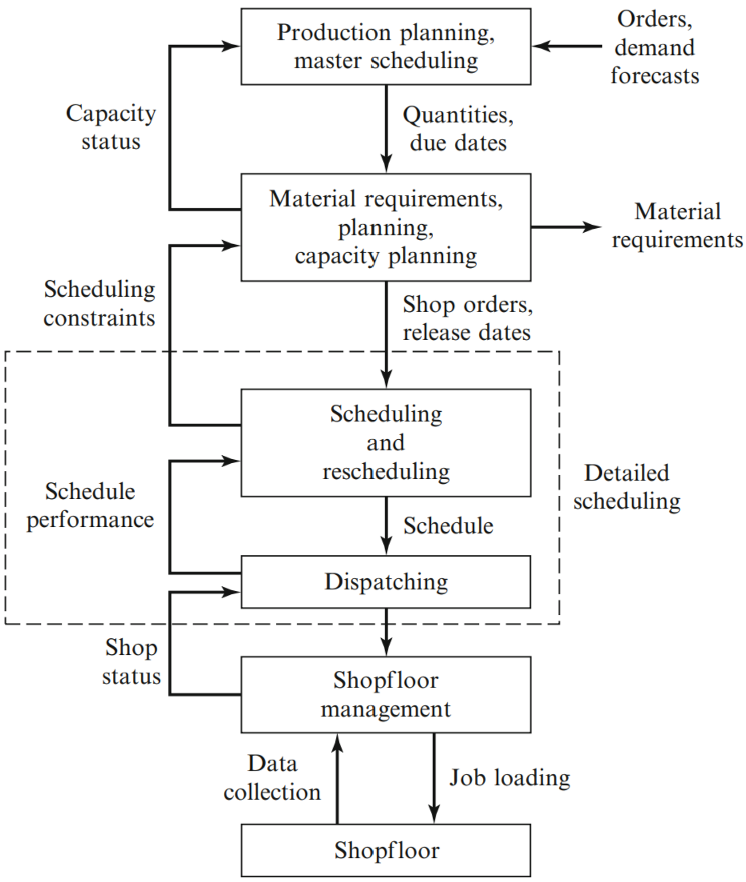

Figure 2.1: Information flow diagram in a manufacturing system

In the petrochemical sector — the focus of this study — given the complexity of resin or plastic production [14], several applications of planning models have already been identified, particularly in refineries [17]. According to Mrad and Alfares [14], in order to maximize profits, production and inventory decisions must be optimized jointly, in an integrated manner. This point is also emphasized by Cooke and Rohleder [6], who highlights the risks of implementing an inventory reduction program without a full understanding of its implications on production performance and customer satisfaction. Thus, integrating inventory control with production planning becomes essential. Meanwhile, Tousain and Bosgra [18] expands this concept to the entire internal supply chain as shown in the Figure 2.2, stating that, in order to operate responsively to the market, internal alignment across the organization is necessary. Furthermore, the ability to model over multiple periods is highly valued, as demonstrated in the Texaco case study by Rigby et al. [19].

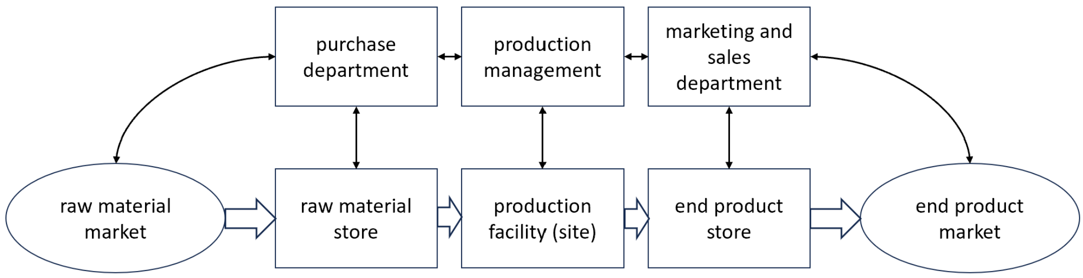

Figure 2.2: Supply chain model for a continuous chemical manufacturing site

The following section details two closely related aspects of production planning: scheduling and lot-sizing. While scheduling focuses on the sequencing and scheduling of production activities, lot-sizing emphasizes determining the optimal quantities and timing of production. In the mathematical model developed in this study to address such a complex problem, both concepts are fundamental to achieve an effective and practical solution.

2.2.1 Scheduling

According to Baker and Trietsch [20], scheduling theory is primarily concerned with mathematical models related to the scheduling process. In the academic domain, these models are classified based on the configuration of resources and the nature of the tasks.

In this type of problem, two types of feasibility constraints are commonly encountered. The first is machine capacity, which reflects the availability of resources, and the second is the technological constraint related to the production order of the jobs. By satisfying both constraints and staying within the feasible region, solving a scheduling problem can be summarized as answering two key questions: which resource should be allocated to perform each task, and when each task should be executed [20].

A common visualization tool used in these problems is a Gantt chart, which shows resource allocation of the task in a horizontal linear temporal axis. In the Figure 2.3, it shows an example of a Gantt chart considering the allocation of four jobs into three resources.

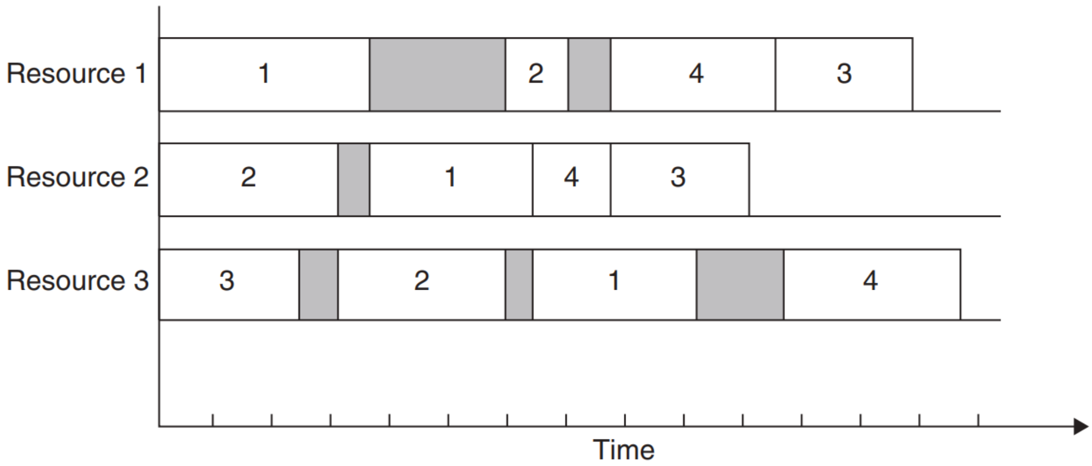

Figure 2.3: Gantt chart representation of scheduling

In the case of petrochemical plants, according to Tousain and Bosgra [18], most multi-grade facilities still operate with a pre-established sequence. This sequence is designed so that transitions are relatively easy, safe, and familiar to operators. However, this practice is now considered inadequate for operating in today's dynamic and competitive markets. Therefore, it reinforces the growing need for increasingly robust and flexible scheduling methods to meet contemporary demands.

Sequencing

A pure sequencing problem is a specialized type of scheduling problem in which the ordering of tasks entirely determines the schedule [20]. Still according to Baker and Trietsch [20], a basic problem of this type is the single-machine problem, meaning it involves only one machine as a resource. Additionally, it is generally characterized by the following conditions:

- Condition 1 – All n tasks are simultaneously available for processing at time zero;
- Condition 2 – Machines can process at most one task at a time;

- Condition 3 – Setup times for the tasks are independent of the sequencing and are included in the processing time;
- Condition 4 – Task descriptions are deterministic and known in advance;
- Condition 5 – Machines are continuously available (no breakdowns and 100% efficiency);
- Condition 6 – Machines will never be idle as long as there are tasks in the queue;
- Condition 7 – No interruption or preemption is allowed once a task has started.

2.2.2 Lot-sizing

Lot-sizing problems aim to determine when and how much of a product should be produced in order to minimize setup, production, and inventory costs.

The application of this type of problem is quite widespread in operations such as forging, casting, and industries where production processes can be considered as a single operation, as is the case in the chemical and pharmaceutical industries [21].

In its simplest form — featuring a single level of production planning, a finite time horizon, deterministic demand, and no inventory carryover — the lot-sizing problem mainly consists of determining when and how much to produce [21]. On the other hand, in its more general form, lot-sizing problems become significantly more complex, involving not only the timing, quantity, and sequencing of production lots for final products, but also for all the components that constitute them. Additionally, they must account for variable demands that compete for limited and scarce resources [16].

According to Karimi et al. [21], solution methods for this type of problem can be categorized into three main groups in the literature: exact methods, common-sense or specialized heuristic methods, and finally, programming-based heuristics.

Capacitated lot-sizing

Within the field of lot-sizing, several branches have emerged, leading to a variety of research subcategories. These can be broadly summarized and categorized as follows [21]:

- Single-level lot-sizing: Focuses on demand variation over the planning horizon;
- Multi-level lot-sizing: Emphasizes the dependencies and relationships among components within a multi-level product structure;

- Capacitated lot-sizing: Addresses prioritization issues caused by limited production capacity;

- Economic lot scheduling: Focuses on incorporating sequencing decisions into lot-sizing problems.

The following section presents a generic model from Karimi et al. [21] for single-level capacitated lot-sizing, which provides fundamental knowledge for further exploration later on.

Assumptions and premises:

- Finite time horizon;

- Deterministic dynamic demand;

- Inventory cost is proportional to the quantity and duration of storage;

- Linear production cost;

- Fixed setup cost, independent of sequencing.

Table 2.1: Indexes and Sets of the Single-Level Capacitated Lot-Sizing Model

Elements	Description
$i \in I$	Where i is the index representing each item, and I is the set of all items.
$t \in T$	Where t is the index representing each time period, and T is the set of all time periods.

Table 2.2: Parameters of the Single-Level Capacitated Lot-Sizing Model

Elements	Description
R_t	Available capacity in time period t
$d_{i,t}$	Demand of item i in time period t
$C_{i,t}$	Unit production cost of item i in time period t.
$S_{i,t}$	Setup cost if item i is produced in time period t.
a_i	Unit resource consumption for item i.
$h_{i,t}$	Inventory holding cost of item i at the end of time period t.

Decision variables:

$$X_{i,t} = \text{Production quantity of item } i \text{ in time period } t. \tag{2.1}$$

$$I_{i,t} = \text{Inventory quantity of item } i \text{ at the end of time period } t. \tag{2.2}$$

$$Y_{i,t} = \begin{cases} 1, & \text{if item } i \text{ is produced in time period } t. \\ 0, & \text{otherwise} \end{cases} \tag{2.3}$$

Objective function:

$$Minimize\ Z = \sum_{i=1}^{n}\sum_{t=1}^{T}(S_{i,t} * Y_{i,t} + C_{i,t} * X_{i,t} + h_{i,t} * I_{i,t}) \tag{2.4}$$

Constraints:

$$\sum_{i=1}^{n} a_i * X_{i,t} \leq R_t,\ t \in T \tag{2.5}$$

$$X_{i,t} + I_{i,t-1} - I_{i,t} = d_{i,t},\ i \in n,\ t \in T \tag{2.6}$$

$$X_{i,t} \leq M_{i,t} * Y_{i,t},\ i \in n,\ t \in T \tag{2.7}$$

$$Y_{i,t} \in \{0,1\},\ i \in n,\ t \in T \tag{2.8}$$

$$X_{i,t} \geq 0,\ i \in n,\ t \in T \tag{2.9}$$

$$I_{i,t} \geq 0,\ i \in n,\ t \in T \tag{2.10}$$

The objective function (2.4) in this model consists of the summation of three terms. The first term represents the total setup cost, while the second term accounts for the production cost of items i. Finally, the third and last term represents the inventory holding cost of items i at the end of the time period t.

On the other hand, the six constraints of the model are detailed as follows:

- Capacity constraint (2.5) limits the total production of lots, ensuring it does not exceed the maximum available capacity;
- Inventory balance constraint (2.6) ensures mass balance in the system between production, inventory, and demand;

- Production enforcement constraint (2.7) forces the variable $Y_{i,t}$ to be greater than or equal to 1 if $X_{i,t}$ takes on a positive integer value. In other words, if there is a positive production quantity of a given "grade", it ensures that the item is indeed produced at the plant;
- Binary variable constraint (2.8) guarantees the binary nature of the variable $Y_{i,t}$;
- Non-negativity constraint for production (2.9) ensures that the production quantity variable $X_{i,t}$ assumes a non-negative value;
- Non-negativity constraint for inventory (2.10) ensures that the inventory variable $I_{i,t}$ assumes a non-negative value.

2.3 Research gap addressed

With the growing complexity of production systems, it has become evident that industrial practices increasingly require not just technical knowledge of a single research subcategory, but rather a combination of them. The interactions within a multi-level structure can significantly influence the feasible solutions due to limited resource capacity. Similarly, poor lot sequencing that disregards setup costs can negatively impact line efficiency, causing disruptions and misalignment between planning and actual production performance — particularly in terms of lead times. Given this, the mathematical model presented in this work aims to bridge and connect lot-sizing with scheduling, then apply it to a real-world problem in order to address the existent challenges faced by the company in question. In other wrods, this thesis has focused on investigating all of these elements together, targeting to understand the interactions between them and apply a mixed-integer linear programming model to effectively address the problem.

Chapter 3

Mathematical Modeling

Given the challenges and specific characteristics of petrochemical production — which exhibits features of continuous production using a single machine — it becomes evident that the central issue is flexibility to adapt to the dynamic demands of the market. Thus, one of the core technological priorities is the development of a decision support system capable of managing the key decisions within the internal supply chain (purchasing, production, and sales) in an integrated manner. This system must ensure consistency between marketing, purchasing, and sales on one side, and production control on the other [18]. The following model is designed to fulfill this role by addressing these requirements and meeting the specific needs of the company in question.

The mathematical formulation used for the problem in question is the same as introduced in Abdullah et al. [22]. The following sections will first present the assumptions, the indexes of the model, the parameters, and the decision variables to provide an initial understanding of the algorithm's scope as well as its limitations. Next, the objective function and the constraints will be detailed, showing how they interact and are connected to define the feasible region and search for the optimal solution.

3.1 Transforming the Chemical Process to the Production Conceptual Model

As shown in Figure 1.3, although the chemical process is quite complex — involving various material inputs and the need to control and monitor reaction conditions such as temperature and pressure — from a production standpoint, this process can be simplified in its operational modeling. In the present work, since the scope emphasizes lot-sizing and sequencing, the input materials will be simplified. Moreover, consumable materials such as catalysts and additives will not be considered, given the abundance of these resources and their immediate availability within the company for processing. Finally, the physicochemical conditions of the reactions are also excluded from the formulation, assuming ideal operation due to the constant monitoring and control carried out by the chemical engineering team. Thus, the production process can be summarized as continuous production; single-machine; and single-level product, as illustrated in Figure 3.1.

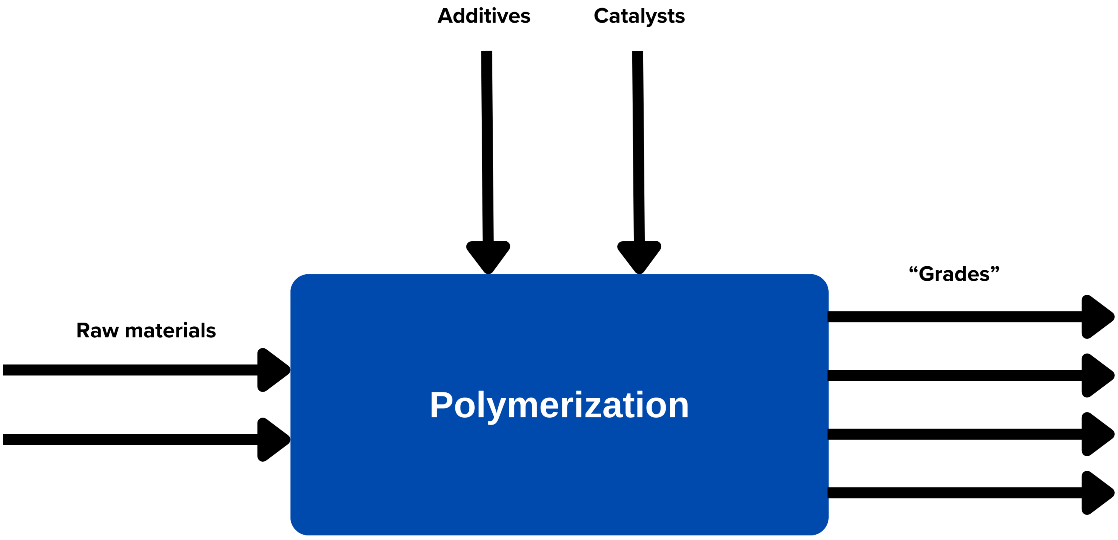

Figure 3.1: Diagram of production process

3.2 Notation

The following sections will detail, in order, the assumptions and premises, as well as the indexes, sets, and parameters of the model. Finally, the decision variables are presented.

Assumptions and premises:

- Each supplier has a limited capacity: the availability of raw material is limited;
- Production is made in several plants: flexibility of production facilities;
- Each plant has a limited capacity: the production at each plant is constrained;
- Each plant may produce all the "grades": production facilities are uniform;
- Each "grade" has different profit per unit: product differentiation in terms of value;

- Each "grade" has different demand: differentiation based on market needs and product usage;
- All "grades" use the same type of raw material: raw material simplification;
- All "grades" has the same usage of raw material consumption rate: standardization of production input usage;
- Demand must be satisfied unless unfeasible: ensuring customer satisfaction;
- Inventory is allowed at production plants: inventory inclusion in the modeling;
- Inventory is not allowed at consolidation points: consolidation points act as transfer nodes;
- All "grades" need to be transported to the consolidation points then to the customers: flexibility in transportation logistics;
- The production can start from any grade each time unit: discontinuity between months in terms of production sequence;
- No carry-over setup is allowed: machine reconfiguration occurs between time periods.

A summary of the assumptions and premises is presented in Table 3.1. Additionally, hypotheses that are also adopted in other academic studies are highlighted on the right-hand side as references.

As shown in the Table 3.1, the premises used in Abdullah et al. [22] can be classified into three categories: common-sense assumptions, industry standards, and problem-specific assumptions. The first two categories are well-supported by the literature, with several studies adopting similar premises. However, the third category does not present any meaningful theoretical background and lacks substantial academic references. Thus, these premises are considered specific to the problem addressed in this study and particular to this modeling. Therefore, any misalignment between the real case in study and these assumptions requires careful analysis and further investigation.

Following the assumptions and premises for this Thesis modeling, Tables 3.2 and 3.3 show the indexes, the sets and the parameters used.

Table 3.1: Assumptions and premises for this Thesis modeling

Nº	Assumptions from Abdullah et al. [22]	Other literature references
1	Each supplier has a limited capacity	Alqahtani et al. [7]* Alfares [23]* Tjoa et al. [4]*
2	Production is made in several plants	Alfares [23]
3	Each plant has a limited capacity	Alqahtani et al. [7]* Alfares [5] Joly et al. [24]* Ghaithan [2]
4	Each plant may produce all the "grades"	Alqahtani et al. [7]*
5	Each "grade" has different profit per unit	Alfares [23] Cooke and Rohleder [6]*
6	Each "grade" has different demand	Alqahtani et al. [7] Alfares [23] Joly et al. [24] Ghaithan [2] Pontes et al. [25] Tjoa et al. [4] Cooke and Rohleder [6] Prata et al. [26]
7	All "grades" use the same type of raw material	Ghaithan [2]
8	All "grades" have the same usage of raw material	Alqahtani et al. [7]* Prata et al. [26]*
9	Demand must be satisfied unless unfeasible	Alqahtani et al. [7]* Alfares [5]
10	Inventory is allowed at production plants	Alqahtani et al. [7] Ghaithan [2]* Cooke and Rohleder [6]*
11	Inventory is not allowed at consolidation points	Joly et al. [24]
12	All "grades" need to be transported to the consolidation points then to the customers	-
13	The production can start from any "grade" each time unit	-
14	No carry-over setup is allowed	-

*Note: * Indicates adaptations of the assumptions and premises made by the respective authors in their studies. In other words, do not match exact statements from Abdullah et al. [22].*

Table 3.2: Indexes and Sets of this Thesis Model

Elements	Description
$g \in G$	Where g is the index representing each supplier, and G is the set of all suppliers.
$i \in I$	Where i is the index representing each production plant. and I is the set of all production plants.
$j, h \in J$	Where j and h are the indices representing each "grade", and J is the set of all "grades".
$e \in E$	Where e is the index representing each consolidation point, and E is the set of all consolidation points.
$k \in K$	Where k is the index representing each customer. and K is the set of all customers.
$t \in T$	Where t is the index representing each time period. and T is the set of all time periods.

Table 3.3: Parameters of this Thesis Model

Parameters	Description
S_g	Supply capacity of supplier g
A_i	Production capacity of plant i
$C_{i,j,t}$	Production cost of "grade" j at plant i during time period t
$N_{i,j,t,h}$	Production cost of "off-grade" resulting from the transition between "grades" j and h at plant i during time period t
$O_{i,j,h,t}$	Production quantity of "off-grade" resulting from the transition from "grade" j and h at plant i during time period t
$H_{i,j,t}$	Inventory cost of "grade" j at plant i during time period t
$D_{k,j,t}$	Demand for "grade" j by customer k during time period t
$C_{1_{g,i,t}}$	Unit transportation cost of raw material from supplier g to plant i during time period t
$C_{2_{i,j,e,t}}$	Unit transportation cost of "grade" j from plant i to consolidation point e during time period t
$C_{3_{e,j,k,t}}$	Unit transportation cost of "grade" j from consolidation point e to customer k during time period t
M	A very large number

Decision variables:

$$x_{i,j,t} = \begin{array}{l}\text{Quantity of "grade" } j \text{ produced at plant } i \text{ during} \\ \text{during time period } t\end{array} \tag{3.1}$$

$$I_{i,j,t} = \begin{array}{l}\text{Inventory level of "grade" } j \text{ stored at plant } i \\ \text{at the end of time period } t\end{array} \tag{3.2}$$

$$y_{i,j,t} = \begin{cases} 1, & \text{If "grade" } j \text{ is produced at plant } i \\ & \text{during time period } t \\ 0, & \text{otherwise} \end{cases} \tag{3.3}$$

$$f_{i,j,t} = \begin{cases} 1, & \text{If a "grade" higher than "grade" } j \text{ is produced at plant } i \\ & \text{during time period } t \\ 0, & \text{otherwise} \end{cases} \tag{3.4}$$

$$z_{i,j,h,t} = \begin{cases} 1, & \text{If there is a transition between grades } j \text{ and } h \text{ at plant } i \\ & \text{during time period } t \\ 0, & \text{otherwise} \end{cases} \tag{3.5}$$

$$SA_{g,i,t} = \begin{array}{l}\text{Quantity of raw material transported from supplier } g \\ \text{to plant } i \text{ during time period } t\end{array} \tag{3.6}$$

$$AW_{i,j,e,t} = \begin{array}{l}\text{Quantity of "grade" } j \text{ transported from plant } i \text{ to consolidation} \\ \text{point } e \text{ during time period } t\end{array} \tag{3.7}$$

$$WC_{e,j,k,t} = \begin{array}{l}\text{Quantity of "grade" } j \text{ transported from consolidation point } e \\ \text{to customer } k \text{ during time period } t\end{array} \tag{3.8}$$

3.3 Objective Function and Constraints

Regarding the structure of this section, the objective function and constraints are first presented — properly numbered — and subsequently, the role of each equation in the construction of the model is discussed.

Objective Function:

$$Minimize\ Z = \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{t=1}^{T}(C_{i,j,t} * x_{i,j,t}) + \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{h\geq j+1}^{J}\sum_{t=1}^{T}(N_{i,j,h,t} * O_{i,j,h,t} * z_{i,j,h,t}) +$$

$$+ \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{t=1}^{T}(H_{i,j,t} * I_{i,j,t}) +$$

$$+ \sum_{g=1}^{G}\sum_{i=1}^{I}\sum_{t=1}^{T}(C1_{g,i,t} * sa_{g,i,t}) + \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{e=1}^{E}\sum_{t=1}^{T}(C2_{i,j,e,t} * aw_{i,j,e,t}) +$$

$$+ \sum_{e=1}^{E}\sum_{j=1}^{J}\sum_{k=1}^{K}\sum_{t=1}^{T}(C3_{e,j,k,t} * aw_{e,j,k,t}) \tag{3.9}$$

Constraints:

$$\sum_{i=1}^{I} sa_{g,i,t} \leq S_g,\ g \in G,\ t \in T \tag{3.10}$$

$$\sum_{j=1}^{J} x_{i,j,t} + \sum_{j=1}^{J}\sum_{h\geq j+1}^{J}(o_{i,j,h,t} * z_{i,j,h,t}) \leq A_i,\ i \in I,\ t \in T \tag{3.11}$$

$$\sum_{e=1}^{E} wc_{e,j,k,t} = D_{j,k,t},\ j \in J,\ k \in K,\ t \in T \tag{3.12}$$

$$\sum_{i=1}^{I} aw_{i,j,e,t} - \sum_{k=1}^{K} wc_{e,j,k,t} = 0,\ j \in J,\ e \in E,\ t \in T \tag{3.13}$$

$$\sum_{g=1}^{G} sa_{g,i,t} = \sum_{j=1}^{J} x_{i,j,t},\ i \in I,\ t \in T \tag{3.14}$$

$$x_{i,j,t} + I_{i,j,t-1} = \sum_{e=1}^{E} aw_{i,j,e,t} + I_{i,j,t},\ i \in I,\ j \in J,\ t \in T \tag{3.15}$$

$$x_{i,j,t} \leq M * y_{i,j,t},\ i \in I,\ j \in J,\ t \in T \tag{3.16}$$

$$x_{i,j,t} \geq y_{i,j,t},\ i \in I,\ j \in J,\ t \in T \tag{3.17}$$

$$\sum_{h\geq j+1}^{J} y_{i,h,t} \leq M * f_{i,j,t},\ i \in I,\ j \in J,\ t \in T \tag{3.18}$$

$$\sum_{h \geq j+1}^{J} y_{i,h,t} \geq f_{i,j,t},\ i \in I,\ j \in J,\ t \in T \tag{3.19}$$

$$z_{i,j,h,t} \leq 0{,}5 * (y_{i,j,t} + y_{i,h,t}),\ i \in I,\ j \in J,\ h \in J,\ t \in T \tag{3.20}$$

$$\sum_{h \geq j+1}^{J} z_{i,j,h,t} \geq y_{i,j,t} + f_{i,j,t} - 1,\ i \in I,\ j \in J,\ t \in T \tag{3.21}$$

$$\sum_{j=1}^{h} z_{i,j,h,t} \leq 1,\ i \in I,\ h \in J,\ t \in T \tag{3.22}$$

The objective function consists of the sum of six terms: the first two are associated with production costs, the third corresponds to inventory holding costs, and the last three are related to transportation costs. The terms included in the objective function (3.9) are detailed below.

- The 1st term represents the total production cost of the grades;
- The 2nd term represents the total production cost of the "off-grades", which can also be interpreted as the transition cost between "grades";
- The 3rd term represents the total inventory cost, or total storage cost, of the "grades" at the production plants;
- The 4th term represents the total transportation cost of raw materials from the suppliers to the production plants;
- The 5th term represents the total transportation cost of the "grades" produced at the plants to the consolidation points;
- The 6th and final term represents the total transportation cost of the grades from the consolidation points to the customers.

On the other hand, the constraints are represented by 13 terms, which are detailed below:

- The supplier capacity constraint (3.10) limits the total raw material supplied to all plants to be less than or equal to the supplier's capacity, for each supplier g and time period t;
- The plant capacity constraint (3.11) limits the production of both "grades" and "non-prime grades" to be less than or equal to the production capacity of each plant i in each time period t;

- The customer demand constraint (3.12) equates the quantity leaving the consolidation points with the customer demand, for each grade i, customer k, and time period t;

- The consolidation point constraint (3.13) equates the quantity of products arriving with the quantity of products leaving, for each grade j, customer k, and time period t;

- The transportation constraints (3.14) and (3.15) ensure mass balance within the system:

  – Constraint (3.14) equates all raw material entering the reactor with the products leaving it, for each plant i and time period t;

  – Constraint (3.15) equates the quantity produced and the inventory from the previous period with the quantity sold and the quantity stored, for each plant i, grade j, and time period t.

- The remaining constraints primarily ensure the correct sequencing of the solution:

  – Constraint (3.16) forces the variable $y_{i,j,t}$ to be greater than or equal to 1 if the variable $x_{i,j,t}$ takes on a positive integer value. In other words, if there is a positive quantity of a given "grade", this ensures that it is produced at the plant;

  – Constraint (3.17) forces the variable $x_{i,j,t}$ to be greater than or equal to 1 if the variable $y_{i,j,t}$ takes on a positive integer value. In other words, if a given "grade" is produced at the plant, this ensures that its production quantity is positive;

  – Constraint (3.18) forces the variable $f_{i,j,t}$ to be greater than or equal to 1 if the term $\sum_{h \leq j+1}^{J} y_{i,h,t}$ takes on a positive integer value. In other words, if a higher "grade" is produced, this ensures that the transition indicator $f_{i,j,t}$ is positive;

  – Constraint (3.19) forces the term $\sum_{h \leq j+1}^{J} y_{i,h,t}$ to be greater than or equal to 1 if the variable $f_{i,j,t}$ takes on a positive integer value. In other words, if the transition indicator $f_{i,j,t}$ is positive, this ensures the production of any higher-grade product;

  – Constraint (3.20) ensures that the variable $z_{i,j,h,t}$ is positive only if there is production of both "grades" j and h;

  – Constraint (3.21) ensures that at least one transition occurs if two "grades" are produced;

– Constraint (3.22) ensures that only one transition is allowed for each "grade".

An important point to be reiterated in equation (3.15) is the very definition of inventory. As mentioned earlier, inventory is calculated based on the final instance of the time period considered. In other words, it accounts only for the remaining quantity after the shipment of products that meet customer demands within that same period.

In addition, it is also necessary to highlight the indexes h and j, which represent the "grades", as well as the special behavior that h exhibits in relation to j. As mentioned in Section **??**, due to the structure of transition costs, it is common for factories to follow a gradual sequencing strategy and avoid jumping between "grades". Therefore, a simplification adopted in the model was to consider only ascending sequencing within each time period. As a result, the index h exhibits a particular behavior, taking on only values greater than index j.

3.4 Data cleansing

This section outlines the data-cleaning procedures applied to the dataset provided by the company, aimed at enabling a more accurate and comprehensive evaluation of current production practices. Upon reviewing the historical production data, the raw dataset revealed numerous small-volume "grade" productions that, from a production planning perspective, lack meaningful significance. These entries typically result from chemical process variations or human error during input adjustments when transitioning between grades. Such anomalies can distort the analysis and hinder fair comparisons from a scheduling standpoint. To better understand the effects of process parameter variations and to isolate the influence of sequencing decisions, this study categorizes two distinct types of error: execution error and planning error, as detailed below.

$$e = \begin{cases} \text{Execution error: } & \text{deviation between the executed process and} \\ & \text{the scheduling plan due to variations in} \\ & \text{process parameters such as temperature,} \\ & \text{pressure, or raw material characteristics.} \\ \text{Planning error: } & \text{deviation between the executed process and} \\ & \text{the optimal scheduling plan resulting from} \\ & \text{sequence execution decisions.} \end{cases}$$

By defining these two types of errors in the database, this work assumes that execution errors can be associated with anomalies. This rationale is based on the company's current practices, which already aim to minimize execution errors by promptly correcting any deviations, thereby preventing the production of large volumes of inaccurate "grades".

Therefore, a technique known as the interquartile range (IQR) was applied to identify and remove anomaly points from the dataset [27], as illustrated in Figure 3.2. The IQR method was chosen because the focus of this study is not on statistical analysis, and the technique is suitable for measuring variability in both normally and non-normally distributed data, thus making it an obvious choice for an easy and fast way to clean the dataset. As a result, this filtering provided a more accurate estimation of the original and current production plans.

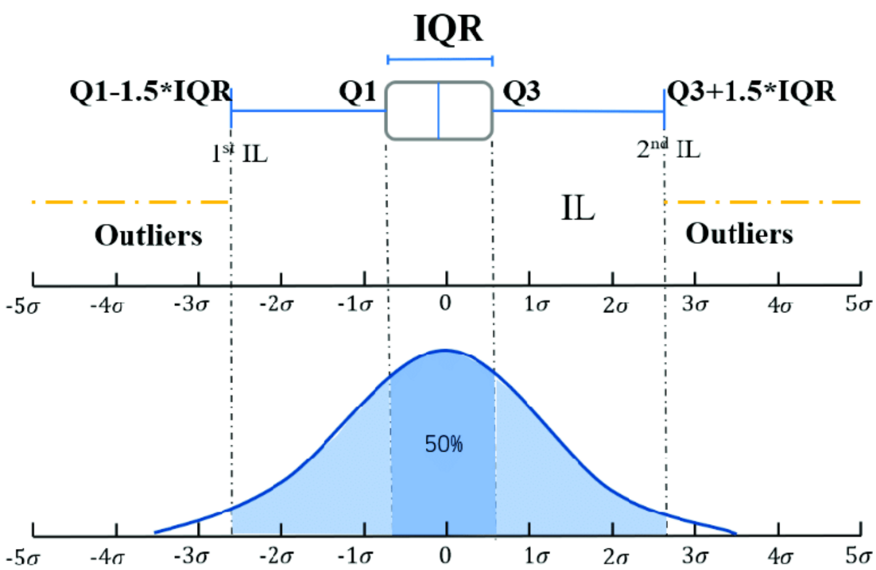

Figure 3.2: Removal of anomaly points using the IQR method

First, it was established the lower and the upper bound based on the calculation of the first and third quartile on top of the available dataset. Then, a range was determined based on those two numbers and any data outside of this range was deemed as an anomaly and cleared out. As a result, cleaner data was obtained to be analyzed without noise. Detailed mathematical formulation can be seen between equation 3.23 and 3.26:

Interquartile Range:

$$Q_1 = \text{First quartile} \tag{3.23}$$

$$Q_3 = \text{Third quartile} \tag{3.24}$$

$$IQR = Q_3 - Q_1 \tag{3.25}$$

$$\text{Outliers} = \begin{cases} \leq Q_1 - 1.5 * IQR \\ \geq Q_3 + 1.5 * IQR \end{cases} \tag{3.26}$$

Chapter 4

Model implementation and Results

This chapter aims to present the implementation process of the model previously described in Section ??, applied to the specific problem addressed in this study. First, the tools used will be explained, along with the execution procedure. Then, certain assumptions and boundary conditions related to the application of the model to the specific problem will be detailed. Finally, the results obtained will be presented, followed by a discussion of their implications.

4.1 Model implementation

The model was developed using the Python programming language in the Visual Studio Code editor, with the support of several complementary tools such as the pandas library, Microsoft Excel, and the Gurobi API (Application Programming Interface) for Python. Figure 4.1 illustrates all the tools used for the model's execution.

Visual Studio Code is a lightweight yet powerful source-code editor that runs on desktop and is available for Windows, macOS, and Linux. It comes with built-in support for several programming languages and features an advanced extension ecosystem for others, such as Python [28]. The algorithm was developed using this editor, which integrates the aforementioned tools into its environment in order to obtain results from the mathematical model.

The choice of the Python programming language is primarily due to the author's prior knowledge and experience with it throughout academic training, as well as its high capability as a system. According to Python Software Foundation [29], Python is an easy-to-learn and powerful language. It has efficient high-level data structures and a simple but effective approach to object-oriented programming.

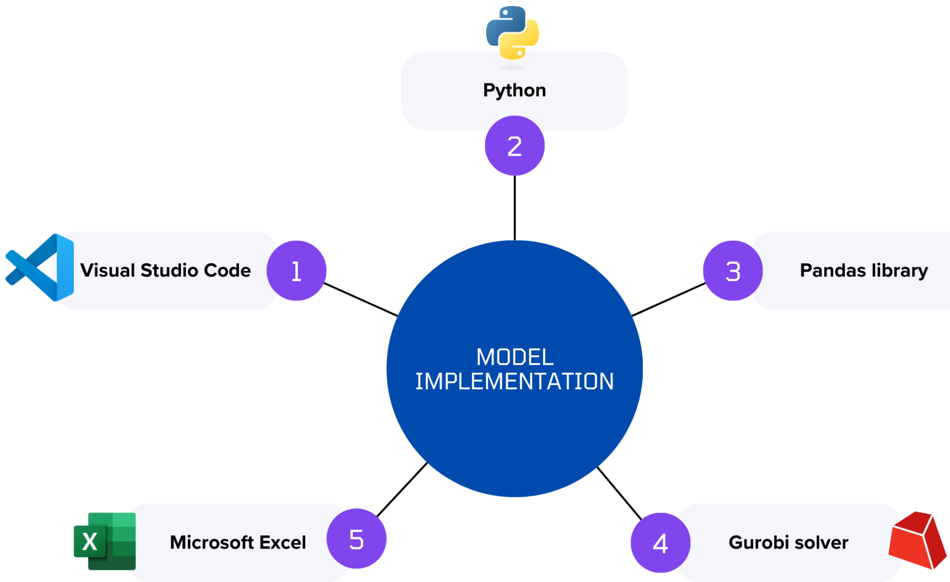

Figure 4.1: Tools for the model implementation

Python's elegant syntax and dynamic typing, combined with its interpreted nature, make it an ideal language for scripting and rapid application development in many areas and across most platforms.

The pandas library is a lightweight, powerful, flexible, and easy-to-use open-source data analysis and manipulation tool built on the Python programming language [30]. In the implemented algorithm, pandas primarily serves as the interface between the Excel spreadsheet and the code. Initially, it extracts the data from the spreadsheet into the programming environment, and later, once the optimal solution is found, the library handles writing the results back into Excel for easier visualization.

Gurobi Optimizer is the fastest solver in the world, offering unmatched performance and support for all major types of optimization problems. It features a lightweight, modern, and intuitive interface that maximizes productivity [31]. Therefore, it is an excellent choice for the present work, given the MILP solution method adopted to address this complex problem.

Finally, Microsoft Excel was used as the primary human interface tool for data analysis, interpretation, and visualization. Both input data and output information are recorded in this program to interface with the algorithm. On one hand, information is entered into the spreadsheets and extracted into the programming environment; on the other hand, the results obtained from the optimizer are written back into the spreadsheet for interpretation and analysis by the human operator. The choice to use this tool was mainly due to its ease of use and widespread adoption — making it an intuitive decision for implementing the model.

Thus, in summary, the input data is recorded in Excel, which is then extracted by the pandas library into the Python environment, where it is processed by the optimizer using the Gurobi solver. Next, the computed results are written back to Excel with the help of pandas, and the entire algorithm was developed and compiled in the Visual Studio Code editor. The algorithm workflow can be represented as shown in the diagram in Figure 4.2.

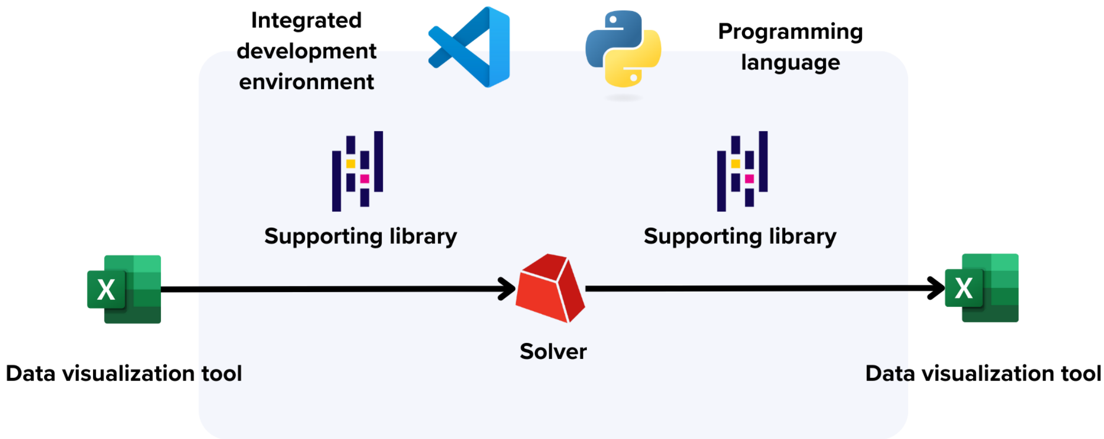

Figure 4.2: Diagram of the tools used in the algorithm

4.1.1 Boundary Conditions of the Implementation

For the implementation and application of the model presented in the Section **??**, several boundary conditions were defined within the scope of the problem, taking into account characteristics and aspects aligned with the specific requirements of the topic. The following section presents the Table 4.1 which summarizes elements and sets defined for the model, along with the rationale behind their selection, based on the operational reality of the company in question.

Table 4.1: Elements and Sets used in the implementation

Sets	# of elements in the set
G	1 supplier
I	1 production plant
J	8 "grades"
E	1 consolidation point
K	1 client
T	5 time periods

The number of suppliers was defined based on the company's current supply chain. As the company is a petrochemical firm that integrates both the first and second generations of thermoplastic resin production, the supply of raw materials for polymerization is internal. That is, the products resulting from first-generation petrochemical reactions are sequentially used within the same company for second-generation processing. Therefore, there is no need for external supply; as a result, the model considers a single supplier. This same simplification can be found in literature as written in the paper by Alqahtani et al. [7].

At the company's request, the initial model proposal considers only a single plant located in Brazil. Thus, although the base model allows for production flexibility across multiple factories, the model is adapted to the specific problem by considering only one plant, where all "grades" are produced.

During discussions with company representatives, it was agreed that the initial focus of the model would be on lot-sizing and scheduling, with the objective of minimizing operational cost by reducing byproduct production. However, there are future plans to expand the scope to a broader supply chain, including consolidation points for finished products as well as their respective customers. With that in mind, the validation of this initial model was focused on answering three core questions: how much to produce, when to produce, and how to sequence production. Therefore, to simplify the implementation, it was established that the model would initially consider only one consolidation point and one customer.

The model considers a fixed time horizon of 5 months, based on the data provided by the company as well as its strategic needs and operational practices. This period was deemed appropriate as it allows the optimization to incorporate the possibility of stockpiling and product storage, aligning with the company's commercial reality. Furthermore, a 5 months planning horizon also meets upper management's requirements for a medium-term perspective, providing transparency and clarity regarding production volumes and expected semiannual revenue.

A conceptual diagram of the implemented model is illustrated in the Figure 4.3.

4.1.2 Model input data

This section details the input data used for the implementation of the model. It begins with information regarding market demand, followed by the inputs related to the production of "grades" and "off-spec" products. Finally, the values related to transportation and inventory across the supply chain are presented.

Table 4.2 shows the market demand for the products. The data was based on information provided by the company and covers the last five time periods. Each "grade" has its own individual demand in each time period, reflecting market demand fluctuations over time.

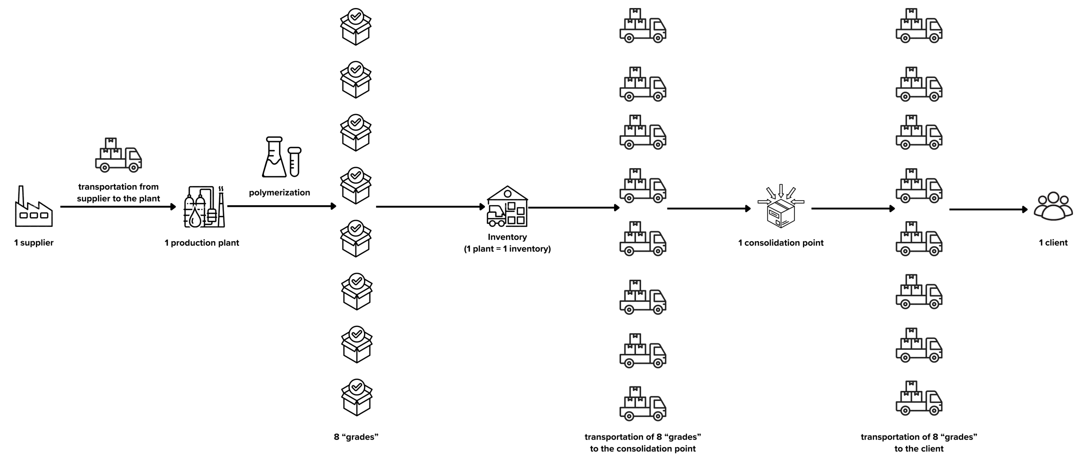

Figure 4.3: Conceptual Diagram of the Implemented Model

Table 4.2: Customer's demands

$D_{i=1,j,t}$	$D_{i=1,j=1,t}$	$D_{i=1,j=2,t}$	$D_{i=1,j=3,t}$	$D_{i=1,j=4,t}$	$D_{i=1,j=5,t}$	$D_{i=1,j=6,t}$	$D_{i=1,j=7,t}$	$D_{i=1,j=8,t}$
$D_{i=1,j,t=1}$	15	72	27	157	117	532	15	38
$D_{i=1,j,t=2}$	262	220	4	97	162	65	0	0
$D_{i=1,j,t=3}$	176	839	228	0	0	0	0	0
$D_{i=1,j,t=4}$	0	0	557	173	58	319	23	0
$D_{i=1,j,t=5}$	0	0	0	33	10	434	84	229

Table 4.3 represents the production cost of the "grades". The values were calculated based on company data and already incorporate the efficiency of the chemical process, considering both the percentage of resin-yielding material in the feedstock and the conversion rate. As evidenced by the differing values, the production of certain resins is more costly than others due to both chemical and operational factors. Additionally, it is assumed that these values remain constant throughout the considered time horizon as the chemical production process of the "grades" is standardized; therefore, the same values are repeated across all five time periods.

Table 4.3: Grades' production cost

$C_{i=1,j,t}$	$C_{i=1,j=1,t}$	$C_{i=1,j=2,t}$	$C_{i=1,j=3,t}$	$C_{i=1,j=4,t}$	$C_{i=1,j=5,t}$	$C_{i=1,j=6,t}$	$C_{i=1,j=7,t}$	$C_{i=1,j=8,t}$
$C_{i=1,j,t=1}$	53	46	47	47	47	62	78	104
$C_{i=1,j,t=2}$	53	46	47	47	47	62	78	104
$C_{i=1,j,t=3}$	53	46	47	47	47	62	78	104
$C_{i=1,j,t=4}$	53	46	47	47	47	62	78	104
$C_{i=1,j,t=5}$	53	46	47	47	47	62	78	104

$H_{i,j,t} = 29.76$ shows the inventory cost of the "grades" at the plants. The values were estimated based on a calculation that considers the cost of warehouse and storage rental in a specific city in Brazil [32] and the average volume of the resins from the company's dataset. In this case, the values are assumed to remain constant throughout the considered time horizon.

$C_{1_{g=1,i,t}} = 1$ represents the cost of transportation from the supplier to the plant. In this case, there is only one internal supplier and minimal value was assumed since this movement occurs internally. Besides, the value remains unchanged during the time horizon considered as the rent cost does not change from one month to another.

$C_{2_{i=1,j,e=1,t}} = 1$ represents the cost of transportation from the plant to the consolidation point. Also in this case, there is only one consolidation point and as before, the minimal value is assumed constant for the very same reason as mentioned above.

$C_{3_{i=1,j,e=1,t}} = 560$ represents the cost of transportation from the consolidation point to the one and only end customers. In order to estimate the cost of transportation to this customer, the geographic location of one of the company's major distributors was used as a reference, and the pricing was obtained via GoFretes [33]. It is worth noting that a simplification was made in the density calculation of the grades, assuming a single value for all transported resins. This simplification was considered acceptable due to the negligible differences in this property among the final products by company's product sheet, which have minimal impact on optimization and final results.

Table 4.4 represents the unit production costs of "off-spec" materials for each time period. The data is based on information provided by the company and remains unchanged over time; therefore, all the tables contain the same values.

Table 4.4: Off-grade's production cost for month 1

$N_{i=1,j,h,t=1}$	$N_{i=1,j,h=1,t=1}$	$N_{i=1,j,h=2,t=1}$	$N_{i=1,j,h=3,t=1}$	$N_{i=1,j,h=4,t=1}$	$N_{i=1,j,h=5,t=1}$	$N_{i=1,j,h=6,t=1}$	$N_{i=1,j,h=7,t=1}$	$N_{i=1,j,h=8,t=1}$
$N_{i=1,j=1,h,t=1}$	0	0	162	160	65	70	77	82
$N_{i=1,j=2,h,t=1}$	0	0	0	0	80	81	89	94
$N_{i=1,j=3,h,t=1}$	160	0	0	0	0	80	92	98
$N_{i=1,j=4,h,t=1}$	80	0	0	0	0	160	123	120
$N_{i=1,j=5,h,t=1}$	80	80	0	0	0	0	200	150
$N_{i=1,j=6,h,t=1}$	70	65	0	0	0	0	0	273
$N_{i=1,j=7,h,t=1}$	86	89	61	123	200	0	0	0
$N_{i=1,j=8,h,t=1}$	80	80	113	113	135	273	0	0

Table 4.5 represents the production quantities of "off-grade" materials for each time period. The data was based on the transition matrix provided by the company and, since this information is inherent to the chemical process, the values remain constant throughout the time horizon considered in the present model.

Table 4.5: Off-grade's production quantity for month 1

$O_{i=1,j,h,t=1}$	$O_{i=1,j,h=1,t=1}$	$O_{i=1,j,h=2,t=1}$	$O_{i=1,j,h=3,t=1}$	$O_{i=1,j,h=4,t=1}$	$O_{i=1,j,h=5,t=1}$	$O_{i=1,j,h=6,t=1}$	$O_{i=1,j,h=7,t=1}$	$O_{i=1,j,h=8,t=1}$
$O_{i=1,j=1,h,t=1}$	0	0	15	15	74	103	133	154
$O_{i=1,j=2,h,t=1}$	0	0	0	0	30	59	88	109
$O_{i=1,j=3,h,t=1}$	15	0	0	0	0	30	59	80
$O_{i=1,j=4,h,t=1}$	30	0	0	0	0	15	44	65
$O_{i=1,j=5,h,t=1}$	60	30	0	0	0	0	15	36
$O_{i=1,j=6,h,t=1}$	103	74	0	0	0	0	0	11
$O_{i=1,j=7,h,t=1}$	118	88	88	44	15	0	0	0
$O_{i=1,j=8,h,t=1}$	158	128	69	69	40	11	0	0

4.2 Results

The algorithm was executed on a personal computer with the configuration specified in Table 4.6 below:

Table 4.6: General information of Personal Computer

Operating System	Windows 11 Home
CPU	Intel(R) Core(TM) i7-1065G7 CPU @ 1.30GHz
Thread count	4 physical cores, 8 logical processors, using up to 8 threads

Some information regarding the model construction, types of variables, and execution time is presented in Table 4.7 below:

Table 4.7: General information about the model

Model	495 rows, 565 columns and 1822 non zeros
Variable type	165 continuous, 400 integers (400 binaries)
Execution time	$\approx$ 0,039s

4.2.1 Model output data

The following section presents the results obtained from the model based on the previously mentioned input data. Starting with the quantity, production, and sequencing of the "grades", the discussion then proceeds to inventory information and, finally, the quantities of raw materials to be purchased, as well as the batch of final products to be delivered to customers.

Table 4.8 shows the quantity of grades to be produced each month, optimized according to the cost-minimization model used. In this case, the determined quantities fully meet the demand for each of the evaluated periods, as expected, achieving 100% market satisfaction.

Table 4.8: Grades' production quantity

$x_{i=1,j,t}$	$x_{i=1,j=1,t}$	$x_{i=1,j=2,t}$	$x_{i=1,j=3,t}$	$x_{i=1,j=4,t}$	$x_{i=1,j=5,t}$	$x_{i=1,j=6,t}$	$x_{i=1,j=7,t}$	$x_{i=1,j=8,t}$
$x_{i=1,j,t=1}$	15	72	27	157	117	532	15	38
$x_{i=1,j,t=2}$	262	220	4	97	162	65	0	0
$x_{i=1,j,t=3}$	176	839	228	0	0	0	0	0
$x_{i=1,j,t=4}$	0	0	557	173	58	319	23	0
$x_{i=1,j,t=5}$	0	0	0	33	10	434	84	229

Table 4.9 is a decision variable that indicates which grades will be produced in a given month. In other words, it determines which products the reactor should be activated for during that production period. The results show consistency between decision variable $x_{i,j,t}$ and variable $y_{i,j,t}$, confirming the correct functioning of the model.

Table 4.9: Grades' production

$y_{i=1,j,t}$	$y_{i=1,j=1,t}$	$y_{i=1,j=2,t}$	$y_{i=1,j=3,t}$	$y_{i=1,j=4,t}$	$y_{i=1,j=5,t}$	$y_{i=1,j=6,t}$	$y_{i=1,j=7,t}$	$y_{i=1,j=8,t}$
$y_{i=1,j,t=1}$	1	1	1	1	1	1	1	1
$y_{i=1,j,t=2}$	1	1	1	1	1	1	0	0
$y_{i=1,j,t=3}$	1	1	1	0	0	0	0	0
$y_{i=1,j,t=4}$	0	0	1	1	1	1	1	1
$y_{i=1,j,t=5}$	0	0	0	1	1	1	1	1

Table 4.10 represents an output that supports the construction of the sequencing logic alongside the decision variable $z_{i,j,h,t}$, but it does not carry any standalone interpretative meaning on its own.

Table 4.10: Grades' auxiliary production variable

$f_{i=1,j,t}$	$f_{i=1,j=1,t}$	$f_{i=1,j=2,t}$	$f_{i=1,j=3,t}$	$f_{i=1,j=4,t}$	$f_{i=1,j=5,t}$	$f_{i=1,j=6,t}$	$f_{i=1,j=7,t}$	$f_{i=1,j=8,t}$
$f_{i=1,j,t=1}$	1	1	1	1	1	1	1	0
$f_{i=1,j,t=2}$	1	1	1	1	1	0	0	0
$f_{i=1,j,t=3}$	1	1	0	0	0	0	0	0
$f_{i=1,j,t=4}$	1	1	1	1	1	1	0	0
$f_{i=1,j,t=5}$	1	1	1	1	1	1	1	0

$I_{i=1,j,t} = 0$ represents the quantity of each grade to be stored for each evaluated time period. As observed, the optimization resulted in a zero inventory policy, indicating that the optimal solution in this specific case is to store no grades at all during any of the months. This outcome may be influenced by several factors, but primarily, it is driven by the constant production cost of the grades in the input data. As a result, the system minimizes total cost by avoiding inventory altogether, since any storage mounts up an additional cost on top of the optimized solution. At the time of being without business' stock information, a realistic outcome and interpretation based on this insight for the company in question is to consider safety stock as a baseline, then avoid any extra inventory on top of the minimum safety quantity in order to minimize the operational cost.

Table 4.11 presents the sequencing results for Month 1. In this period, seven sequential transitions occur from "grade" 1 to "grade" 8. As illustrated in the Table 4.11, the first transition is from "grade" 1 to "grade" 2; therefore, the cell corresponding to row $j = 1$ and column $h = 2$ is assigned the value 1. The same logic is applied to interpret the subsequent transitions throughout the table.

Table 4.11: Transition for the month 1

$z_{i=1,j,h,t=1}$	$z_{i=1,j,h=1,t=1}$	$z_{i=1,j,h=2,t=1}$	$z_{i=1,j,h=3,t=1}$	$z_{i=1,j,h=4,t=1}$	$z_{i=1,j,h=5,t=1}$	$z_{i=1,j,h=6,t=1}$	$z_{i=1,j,h=7,t=1}$	$z_{i=1,j,h=8,t=1}$
$z_{i=1,j=1,h,t=1}$	0	1	0	0	0	0	0	0
$z_{i=1,j=2,h,t=1}$	0	0	1	0	0	0	0	0
$z_{i=1,j=3,h,t=1}$	0	0	0	1	0	0	0	0
$z_{i=1,j=4,h,t=1}$	0	0	0	0	1	0	0	0
$z_{i=1,j=5,h,t=1}$	0	0	0	0	0	1	0	0
$z_{i=1,j=6,h,t=1}$	0	0	0	0	0	0	1	0
$z_{i=1,j=7,h,t=1}$	0	0	0	0	0	0	0	1
$z_{i=1,j=8,h,t=1}$	0	0	0	0	0	0	0	0

Table 4.12 presents the sequencing results for Month 2. In this period, production begins with 'grade' 1 and concludes with "grade" 6. As in the previous case, all transitions are carried out sequentially.

Table 4.12: Transition for the month 2

$z_{i=1,j,h,t=2}$	$z_{i=1,j,h=1,t=2}$	$z_{i=1,j,h=2,t=2}$	$z_{i=1,j,h=3,t=2}$	$z_{i=1,j,h=4,t=2}$	$z_{i=1,j,h=5,t=2}$	$z_{i=1,j,h=6,t=2}$	$z_{i=1,j,h=7,t=2}$	$z_{i=1,j,h=8,t=2}$
$z_{i=1,j=1,h,t=2}$	0	1	0	0	0	0	0	0
$z_{i=1,j=2,h,t=2}$	0	0	1	0	0	0	0	0
$z_{i=1,j=3,h,t=2}$	0	0	0	1	0	0	0	0
$z_{i=1,j=4,h,t=2}$	0	0	0	0	1	0	0	0
$z_{i=1,j=5,h,t=2}$	0	0	0	0	0	1	0	0
$z_{i=1,j=6,h,t=2}$	0	0	0	0	0	0	0	0
$z_{i=1,j=7,h,t=2}$	0	0	0	0	0	0	0	0
$z_{i=1,j=8,h,t=2}$	0	0	0	0	0	0	0	0

Table 4.13 presents the sequencing results for Month 3. In this period, only two transitions occur, with production primarily focused on "grades" 1, 2, and 3. The sequence begins with a transition from "grade" 1 to "grade" 2, followed by a final transition from "grade" 2 to "grade" 3.

Table 4.13: Transition for the month 3

$z_{i=1,j,h,t=3}$	$z_{i=1,j,h=1,t=3}$	$z_{i=1,j,h=2,t=3}$	$z_{i=1,j,h=3,t=3}$	$z_{i=1,j,h=4,t=3}$	$z_{i=1,j,h=5,t=3}$	$z_{i=1,j,h=6,t=3}$	$z_{i=1,j,h=7,t=3}$	$z_{i=1,j,h=8,t=3}$
$z_{i=1,j=1,h,t=3}$	0	1	0	0	0	0	0	0
$z_{i=1,j=2,h,t=3}$	0	0	1	0	0	0	0	0
$z_{i=1,j=3,h,t=3}$	0	0	0	0	0	0	0	0
$z_{i=1,j=4,h,t=3}$	0	0	0	0	0	0	0	0
$z_{i=1,j=5,h,t=3}$	0	0	0	0	0	0	0	0
$z_{i=1,j=6,h,t=3}$	0	0	0	0	0	0	0	0
$z_{i=1,j=7,h,t=3}$	0	0	0	0	0	0	0	0
$z_{i=1,j=8,h,t=3}$	0	0	0	0	0	0	0	0

Table 4.14 presents the sequencing results for Month 4. In this period, production begins with "grade" 3 and proceeds sequentially until "grade" 7. As a result, the transition matrix resembles an identity matrix-like format, with values equal to 1 along the diagonal from top to bottom, left to right, indicating a straightforward sequential flow.

Table 4.14: Transition for the month 4

$z_{i=1,j,h,t=4}$	$z_{i=1,j,h=1,t=4}$	$z_{i=1,j,h=2,t=4}$	$z_{i=1,j,h=3,t=4}$	$z_{i=1,j,h=4,t=4}$	$z_{i=1,j,h=5,t=4}$	$z_{i=1,j,h=6,t=4}$	$z_{i=1,j,h=7,t=4}$	$z_{i=1,j,h=8,t=4}$
$z_{i=1,j=1,h,t=4}$	0	0	0	0	0	0	0	0
$z_{i=1,j=2,h,t=4}$	0	0	0	0	0	0	0	0
$z_{i=1,j=3,h,t=4}$	0	0	0	1	0	0	0	0
$z_{i=1,j=4,h,t=4}$	0	0	0	0	1	0	0	0
$z_{i=1,j=5,h,t=4}$	0	0	0	0	0	1	0	0
$z_{i=1,j=6,h,t=4}$	0	0	0	0	0	0	1	0
$z_{i=1,j=7,h,t=4}$	0	0	0	0	0	0	0	0
$z_{i=1,j=8,h,t=4}$	0	0	0	0	0	0	0	0

Finally, Table 4.15 presents the sequencing results for Month 5. In this period, production begins with "grade" 4 and concludes with "grade" 8. As shown in the table, the final transition occurs from "grade" 7 to "grade" 8, and therefore, the cell at position (*j=7; h=8*) is assigned the value 1.

Table 4.15: Transition for the month 5

$z_{i=1,j,h,t=5}$	$z_{i=1,j,h=1,t=5}$	$z_{i=1,j,h=2,t=5}$	$z_{i=1,j,h=3,t=5}$	$z_{i=1,j,h=4,t=5}$	$z_{i=1,j,h=5,t=5}$	$z_{i=1,j,h=6,t=5}$	$z_{i=1,j,h=7,t=5}$	$z_{i=1,j,h=8,t=5}$
$z_{i=1,j=1,h,t=5}$	0	0	0	0	0	0	0	0
$z_{i=1,j=2,h,t=5}$	0	0	0	0	0	0	0	0
$z_{i=1,j=3,h,t=5}$	0	0	0	0	0	0	0	0
$z_{i=1,j=4,h,t=5}$	0	0	0	0	1	0	0	0
$z_{i=1,j=5,h,t=5}$	0	0	0	0	0	1	0	0
$z_{i=1,j=6,h,t=5}$	0	0	0	0	0	0	1	0
$z_{i=1,j=7,h,t=5}$	0	0	0	0	0	0	0	1
$z_{i=1,j=8,h,t=5}$	0	0	0	0	0	0	0	0

Tables 4.11 to 4.15 show the sequencing order that should be followed for each time period. A gradual behavior can be observed, aimed at minimizing transition costs and the production of off-grades, which aligns with the literature and best industrial practices. In addition to this gradual approach, it is also evident that the model optimizes toward minimizing the number of transitions as much as possible, consequently resulting in a more streamlined and efficient production process.

Table 4.16 directly reflects the quantity of raw material to be acquired in order to enable polymer production as required. In this case, the amount of raw material to be transported to the plant perfectly matches the needs for supporting each monthly resin production determined by the model. The values are identical to the total sum of resin quantities, ensuring that there are neither shortages nor excesses that could lead to additional costs.

Table 4.16: Raw-material's transportation quantity

$sa1_{g=1,i,t}$	$sa1_{g=1,i=1,t}$
$sa1_{g=1,i,t=1}$	973
$sa1_{g=1,i,t=2}$	810
$sa1_{g=1,i,t=3}$	1243
$sa1_{g=1,i,t=4}$	1130
$sa1_{g=1,i,t=5}$	790

Table 4.17 presents the quantity of each "grade" to be transported from the production plant to the consolidation point. In this case, only one production plant and one consolidation point are considered; therefore, a single transportation route is responsible for carrying all the produced grades.

Table 4.17: Grades' transportation quantity to the consolidation point

$aw2_{i=1,j,e=1,t}$	$aw2_{i=1,j=1,e=1,t}$	$aw2_{i=1,j=2,e=1,t}$	$aw2_{i=1,j=3,e=1,t}$	$aw2_{i=1,j=4,e=1,t}$	$aw2_{i=1,j=5,e=1,t}$	$aw2_{i=1,j=6,e=1,t}$	$aw2_{i=1,j=7,e=1,t}$	$aw2_{i=1,j=8,e=1,t}$
$aw2_{i=1,j,e=1,t=1}$	15	72	27	157	117	532	15	38
$aw2_{i=1,j,e=1,t=2}$	262	220	4	97	162	65	0	0
$aw2_{i=1,j,e=1,t=3}$	176	839	228	0	0	0	0	0
$aw2_{i=1,j,e=1,t=4}$	0	0	557	173	58	319	23	0
$aw2_{i=1,j,e=1,t=5}$	0	0	0	33	10	434	84	229

Finally, Table 4.18 represents the quantities to be transported to the customers. In this specific case, since there is no product storage and only a single consolidation point and customer, the values directly reflect market demand and the quantities produced each month. In other words, each final product is transported in its respective month of production to the customer who requested that specific polymer quantity, incurring no additional costs while fully satisfying customer demand.

Table 4.18: Grades' production to the final customer

$wc3_{e=1,j,k=1,t}$	$wc3_{e=1,j=1,k=1,t}$	$wc3_{e=1,j=2,k=1,t}$	$wc3_{e=1,j=3,k=1,t}$	$wc3_{e=1,j=4,k=1,t}$	$wc3_{e=1,j=5,k=1,t}$	$wc3_{e=1,j=6,k=1,t}$	$wc3_{e=1,j=7,k=1,t}$	$wc3_{e=1,j=8,k=1,t}$
$wc3_{e=1,j,k=1,t=1}$	15	72	27	157	117	532	15	38
$wc3_{e=1,j,k=1,t=2}$	262	220	4	97	162	65	0	0
$wc3_{e=1,j,k=1,t=3}$	176	839	228	0	0	0	0	0
$wc3_{e=1,j,k=1,t=4}$	0	0	557	173	58	319	23	0
$wc3_{e=1,j,k=1,t=5}$	0	0	0	33	10	434	84	229

4.2.2 Comparisons

In the following section, Gantt charts are presented and compared for each month individually, illustrating the current practices based on the original dataset, the current solution derived from the cleaned dataset, and the proposed solutions generated by the model.

As shown in Figure 4.4, the company produced all eight grades in the first month, resulting in a total of 24 transitions. Although a generally increasing strategy was adopted — resembling a gradual and ascending transformation — in practice, the process was marked by frequent, small-scale cyclic transitions over a short period, leading to production system inefficiencies. After cleaning the data and excluding the anomaly points, though the number of transitions is reduced to 15, this phenomenon persists, which reflects the possible planning error by adopting a suboptimal scheduling practice as seen in the Figure 4.5. Meanwhile, in Figure 4.6, we can see the optimal solution proposed by the model. In this case, the number of transitions was reduced to seven, and a consistent, gradual sequencing is observed, eliminating the small-scale cyclic changes. As a result, the production process becomes leaner, and any byproduct is minimized.

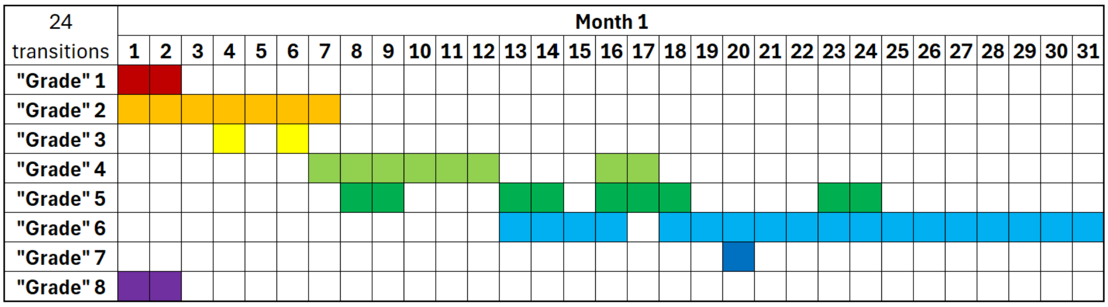

Figure 4.4: Gantt current solution for month 1

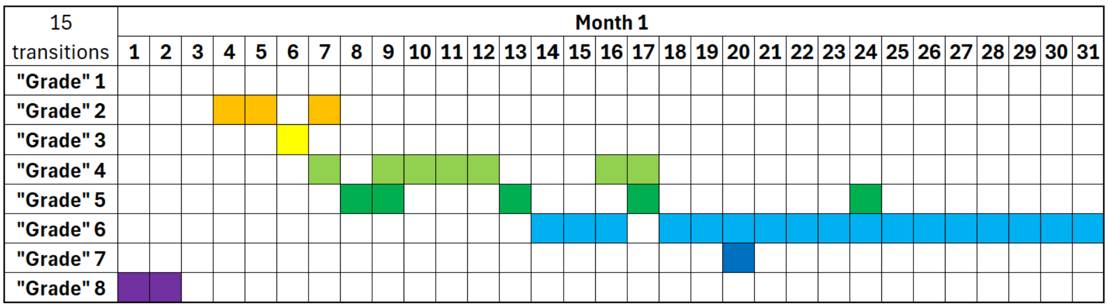

Figure 4.5: Gantt filtered current solution for month 1

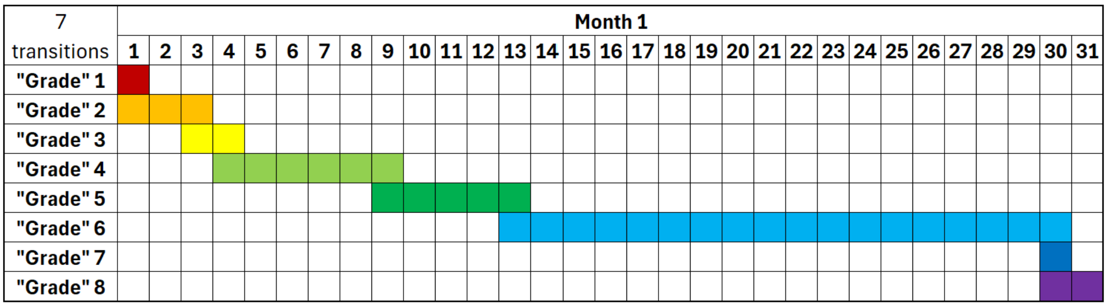

Figure 4.6: Gantt model solution for month 1

Similarly, the same phenomenon can be observed in month 2. Figure 4.7, which reflects the current solution, shows a constant alternation in production between grade 1 and grade 2. This event is highlighted even more in the case of disregarding any possible execution error caused either by chemical abnormalities or operator errors as shown in the Figure 4.8, In contrast, Figure 4.9 eliminates this pattern and replaces it with a single transition between resins, reducing often unnecessary transitions to just five.

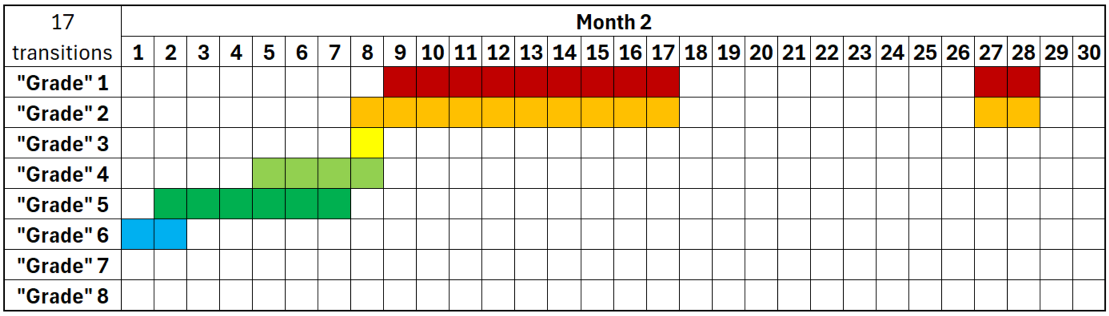

Figure 4.7: Gantt current solution for month 2

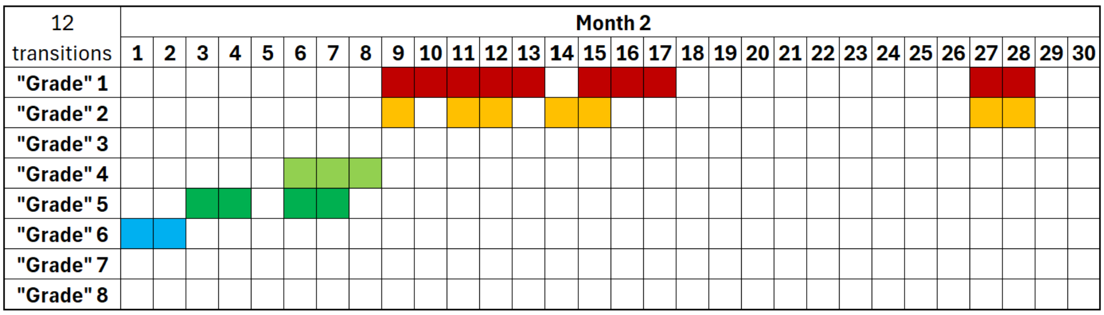

Figure 4.8: Gantt filtered current solution for month 2

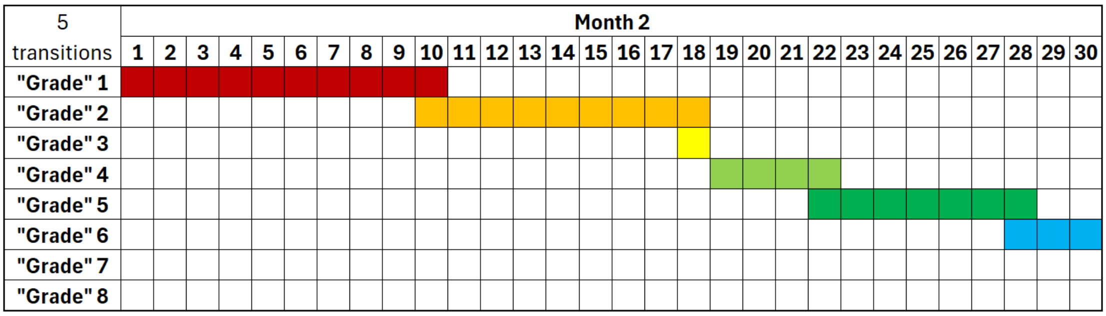

Figure 4.9: Gantt model solution for month 2

In the third month, although only three polymers are produced, the solution in Figure 4.12 chose to organize the transitions sequentially from "grade" 1 to 3, unlike Figures 4.10 and 4.11, which first transitions to "grade" 1 from "grade" 2 and then to "grade" 3. As a result, the new solution was able to reduce the number of transitions from eight to just two during this month.

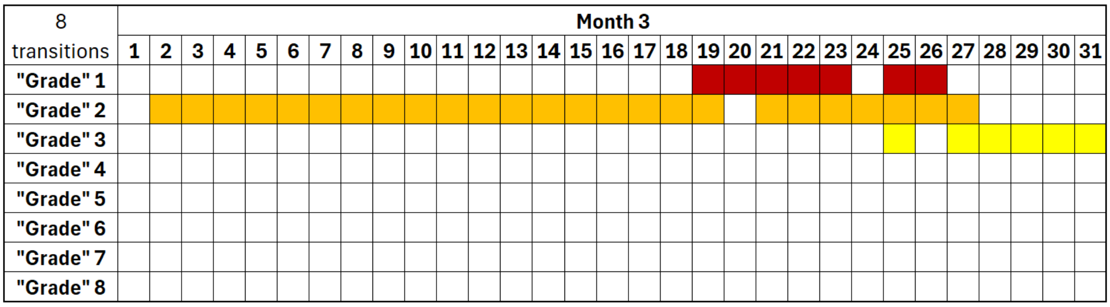

Figure 4.10: Gantt current solution for month 3

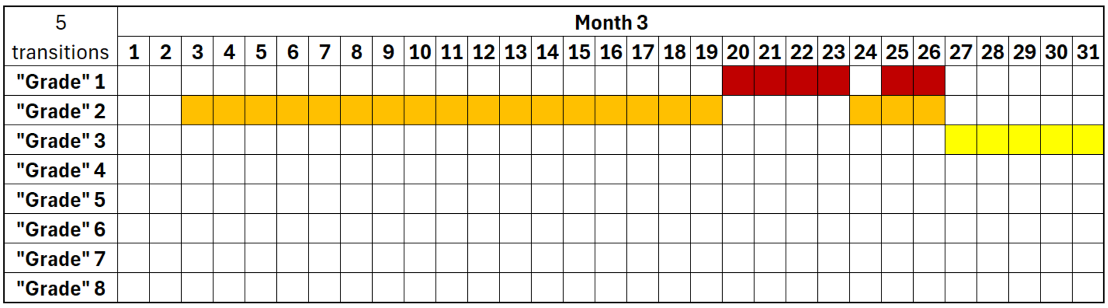

Figure 4.11: Gantt filtered current solution for month 3

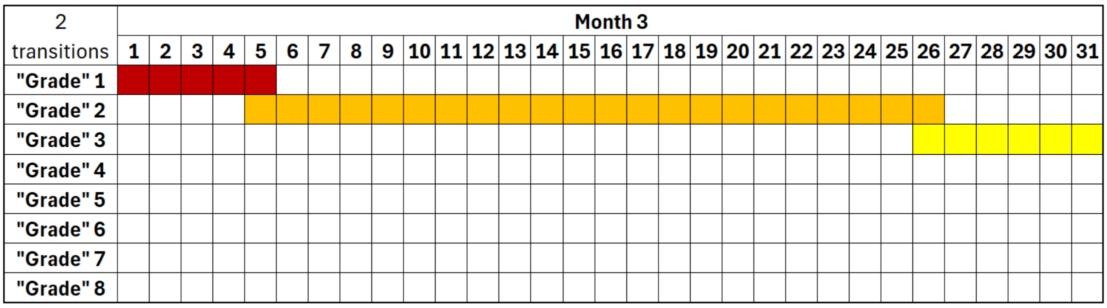

Figure 4.12: Gantt model solution for month 3

In the fourth month, production begins with grade 3 in both solutions, as shown in Figures 4.13 and 4.15. However, instead of performing multiple transitions in a short time frame, the model's solution always prioritizes a single transition within each short interval in order to optimize down-time. As a result, it achieves a total of only 4 transitions during the month, compared to 13 in the existing approach or 6 transitions as in the filtered existing solution.

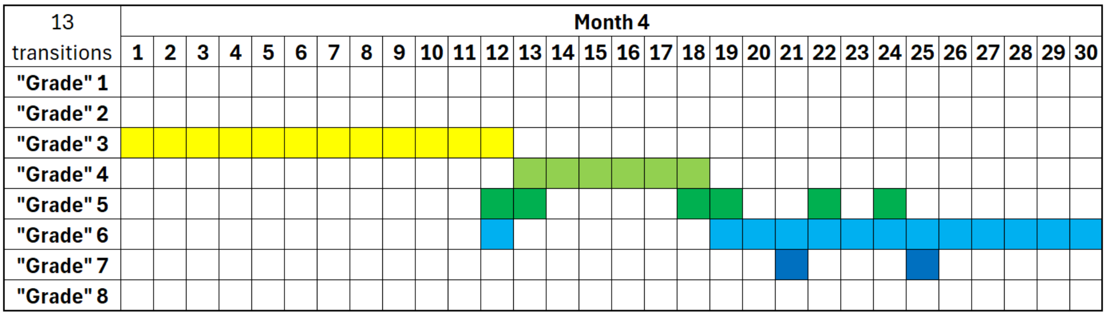

Figure 4.13: Gantt current solution for month 4

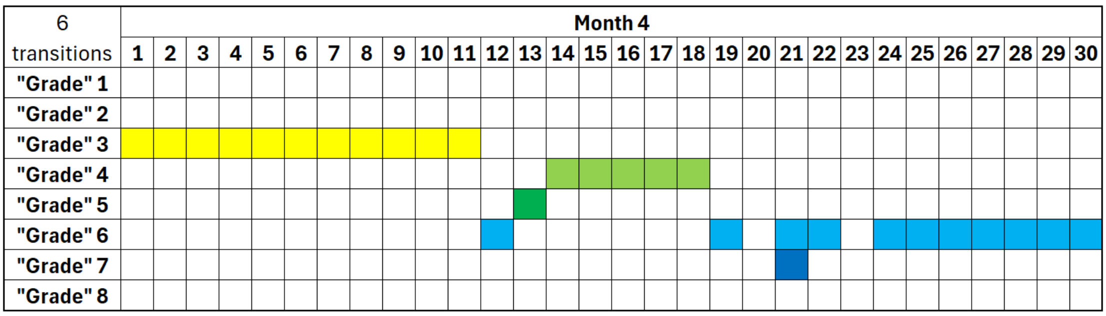

Figure 4.14: Gantt current filtered solution for month 4

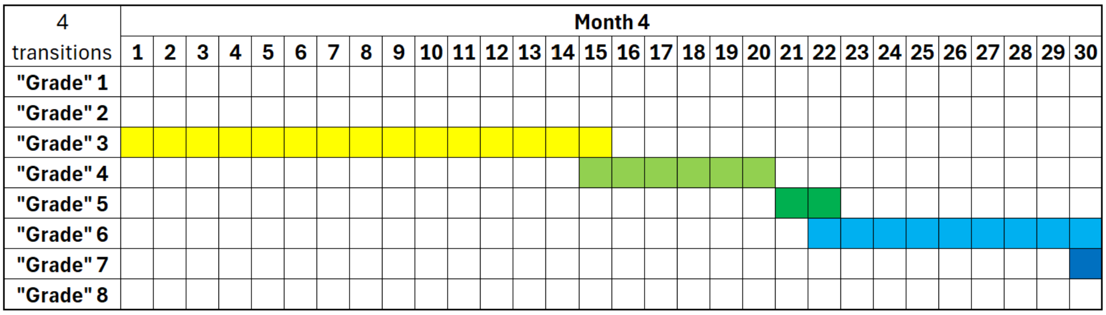

Figure 4.15: Gantt model solution for month 4

Finally, the previous practice in the last month was characterized by somewhat erratic transitions between grades 4 through 8, as shown both in the Figures 4.16 and 4.17. In contrast, the optimized solution in Figure 4.18 demonstrated that it is far more efficient to sequence them in order, reducing the number of transitions to just four.

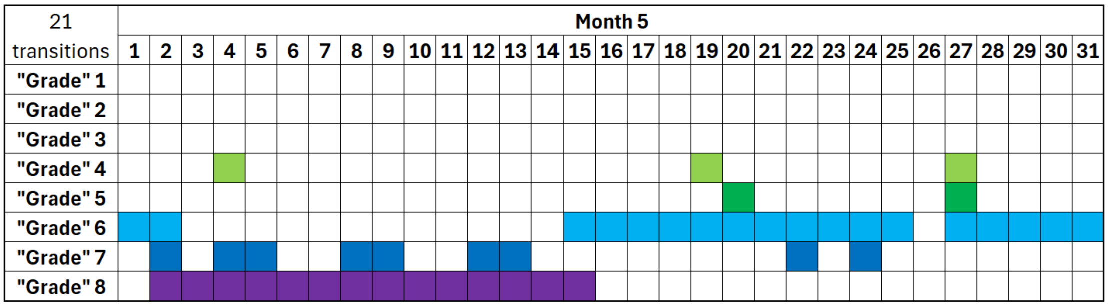

Figure 4.16: Gantt current solution for month 5

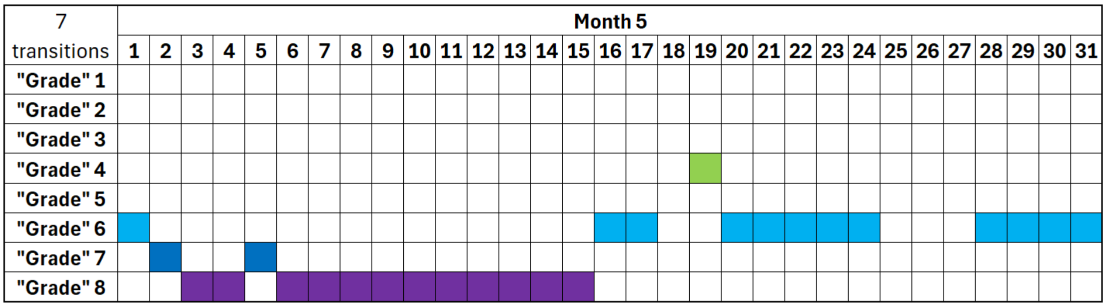

Figure 4.17: Gantt filtered current solution for month 5

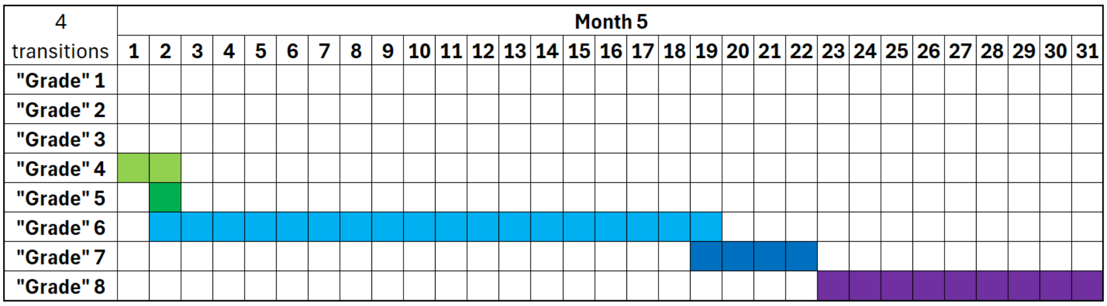

Figure 4.18: Gantt model solution for month 5

A comparative summary of all the solutions can be found in Table 4.19, which includes the objective function values for all the results, as well as the number of transitions per month and their total.

Table 4.19: Comparison summary table

	Current solution	Current filtered solution	Model solution
Objective function	3,109,952	3,073,352	3,052,952
Total number of transitions	83	45	22
Transition month 1	24	15	7
Transition month 2	17	12	5
Transition month 3	8	5	2
Transition month 4	13	6	4
Transition month 5	21	7	4

It is important to emphasize the value of comparing the model's suggested solution with both versions of the current solution — filtered and unfiltered. While the filtered dataset is theoretically more suitable for analyzing and comparing sequencing decisions, the IQR method was applied as a means to infer the original scheduling intent, given the absence of this information from the company. However, this statistical approach generates a dataset free of anomaly points but does not account for the actual executed production plan or real-world operational factors — elements captured in the unfiltered dataset. In other words, the unfiltered dataset presents a complete picture, including execution errors that this study seeks to isolate, whereas the filtered dataset may distort certain aspects by removing data points classified as anomalies. Consequently, both perspectives — filtered and unfiltered — are considered to provide a more comprehensive comparison between the current solution and the optimized one.

Overall, it can be observed between the current solution and the model suggested solution a 1.83% reduction in the objective function — representing the operational cost. Although the percentage may seem small, in absolute terms it speaks for a reduction of 57,000 in less than half a year. On the other hand, a 73.5% decrease in the number of transitions was achieved, which represents 61 fewer transitions in absolute value. When considering the case of filtered data, which represents a more meaningful result for this present work, the gap on the objective function and the number of transitions is shrunk. However, even disregarding the potential execution errors, there is scheduling improvement to make as the optimized result is still the best among the three and brings better sequencing execution decisions. This is also reflected on the objective function, reducing by 20,400 in terms of operational cost in less than half a year.

To better assess the specific impact of the proposed solution on the number of transitions, Figure 4.19 presents a month-by-month comparison of the three scenarios. The current solution clearly results in the highest number of transitions across the entire period analyzed, as it reflects the effects of both execution and planning errors. Even when execution errors are excluded, the optimized solution consistently yields the fewest transitions in each month. This variable directly influences the objective function, which includes the setup and chemical transient state cost. In other words, reducing the number of transitions can have a positive impact on the company's potential financial gains, achieving the ultimate goal for the project on which this work is based.

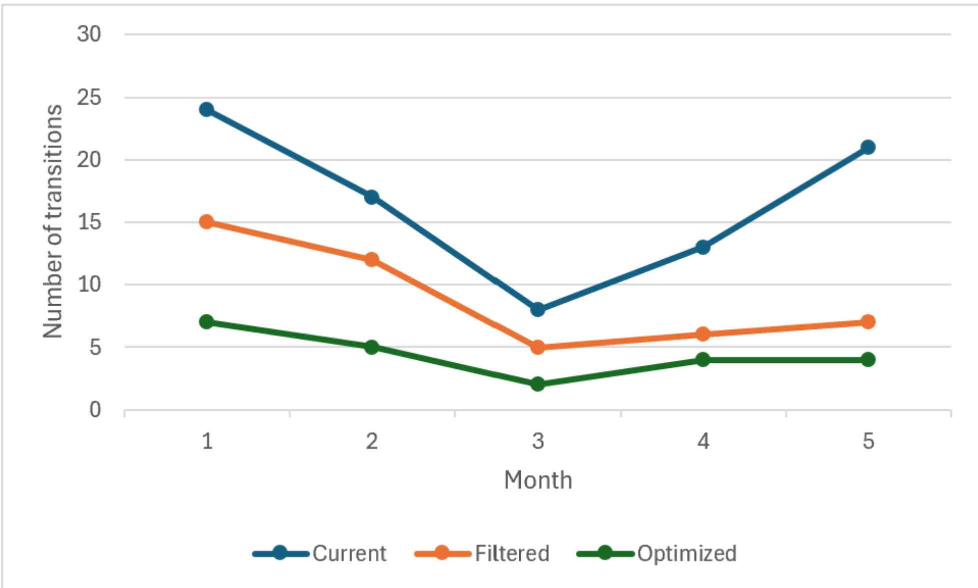

Figure 4.19: Comparison number of transitions

Chapter 5

Conclusion and future works

This study focused on understanding the production process of a petrochemical industry that plays a vital role in both the global economy and contemporary daily life. Based on this, the objective was to reduce operational costs by minimizing "off-spec" byproducts while simultaneously optimizing the production of "grades". By implementing a MILP algorithm, it was possible to obtain an optimal solution using data provided by the company, which demonstrated improvements compared to the organization's current practices. The results highlight the potential of a quantitative approach that integrates various facets of the supply chain, ranging from raw material supply, inventory and lastly, final product delivery to customers.

Through the algorithm, it was possible to determine which "grades" to produce, their monthly production quantities, and their sequencing, while meeting all fundamental requirements. Additionally, it indicated the optimal inventory levels, the required supply of raw materials, the quantity of resins transported to the consolidation point, and their subsequent transportation to the customer. As a result, the findings provide a comprehensive overview of the company's supply chain — from the supplier to the end customer — with a particular focus on lot-sizing and scheduling over a five-month planning horizon.

The solution obtained suggests a reduction in the number of transitions and, consequently, a decrease in costs. This highlights the advantages of prioritizing gradual sequential changes, allowing for a smooth conversion of chemical reactions, as opposed to frequent short-term cyclic transformations that hinder operational efficiency. Through this adjustment, the analyses demonstrated that proper sequencing can lead to a cost reduction in percentage, which translates into a significant impact in absolute value on the company's financial performance.

Although MILP methods present scalability challenges and high computational costs as weaknesses, this study demonstrated that, when properly applied to relevant situations, these techniques can guarantee optimal results that generate valuable reflections and insights for the company's modus operandi. Furthermore, this work advocates for the increasing adoption of quantitative approaches within the petrochemical sector, which continues to grow and become increasingly dynamic in terms of market competitiveness.

5.1 Opportunities for future works

For future works, there is one direction regarding the chemical process itself to be developed: improving the assertiveness of the transitions; and two main directions for the production planning part segment to be developed: improving the model and implementing the solution. In respect of the process assertiveness, improvements on process control could reduce the execution error and guarantee a correct transition. Regarding model improvement, changes can be made both in terms of modifying and expanding boundary conditions to scale the solution, and in terms of enhancing the formulation to achieve a model increasingly aligned with the actual production environment. On the other hand, for solution implementation, efforts should focus on investigating how to incorporate this optimization model into the company's daily operations. This involves considering the existing workflow, the collection and analysis of data to be used as input, and establishing a robust feedback system to support updates and continuous improvement of the model.

Regarding process assertiveness, the installation of additional sensors could significantly enhance process control. The data collected from these devices would provide valuable insights into the influence of input parameters on the production of resin "grades". With this enriched dataset, a simulation model could be developed to replicate production transitions and predict process variations in advance. Additionally, operator training should be conducted in parallel to mitigate human error during operation, thereby improving process control both in terms of chemical reactions and operational execution as a means to reduce the execution error.

In the scope of modifying and expanding the boundary conditions — namely, evaluating the number of elements within the set — it is possible to consider the inclusion of additional consolidation points, more customers, and a greater number of time periods. In this case, it would take into account a more complex internal logistics structure of the company, a broader supply chain, and, finally, a time horizon longer than one semester, thus offering a more strategic and long-term perspective.

Meanwhile, several improvements can be made to the model presented by Abdullah et al. [22] in order to develop a more accurate formulation for the problem at hand. Beginning with the numerical order of the assumptions and premises listed in Section **??**, if additional production plants are to be included — as already anticipated by the company — it is necessary to consider scenarios in which not all "grades" can be produced at every facility. There will be cases where certain plants are specialized and dedicated to specific "grade" families, while others will produce the remaining polymers. A second modification to consider is the assumption that all "grades" use the same raw material. That is, the system considered by the author involves only a single raw material. However, in practice, companies in this sector typically deal with polymerization reactions for a variety of resins, using different raw materials, which requires them to be treated individually. Still regarding assumptions related to raw materials, a more detailed study of the consumption rate of these inputs is necessary — in other words, raw material usage should not be standardized across all production processes. In the specific case of the company in question, it was agreed that the raw material aspect was not a point of concern, since it is supplied internally and stocked abundantly. Lastly, considering the nature of continuous production, the final two assumptions could be revised to better reflect continuity between time periods, especially with respect to setup. In other words, at the beginning of each month, production should take into account the last polymer produced in the previous month and carry that reactor configuration into the current month, given that there is no discontinuity or machine reconfiguration from one month to the next.

Once the assumptions and premises governing the model have been reassessed, a reflection on the formulation of the model itself can follow. In this case, a fundamental issue must be discussed: the modeling of "off-spec" production costs. Starting with the production capacity constraint detailed in the Objective Function (3.9), the cost is calculated by multiplying the quantity of "off-grade" produced by its unit production cost. However, there are many cases in which a transition incurs a cost that is not reflected in tangible material — for example, reactor cleaning, machine setup time, or waiting time — during which the quantity of "off-grade" is zero. In these situations, multiplying a zero quantity by a non-zero cost results in a zero value, thus failing to capture these intangible costs in the current formulation of the model. One possible solution is to dissociate the cost of tangible products from that of intangible operations and to weigh both appropriately in the Objective Function, in order to reflect the real situation more accurately.

It is also important to emphasize the value of considering heuristic methods for solving the problem. As previously mentioned, problems of this type are classified as NP-hard, which leads to high computational costs when the problem is scaled — making exact methods inefficient for finding the optimal solution in such cases. In these situations, a solution approach that approximates sufficiently to optimum with significantly lower computational cost can have a meaningful impact and represent a practical and effective alternative for companies.

Finally, implementing the solution within the company would require a much more collaborative effort from all parties involved. First, a series of more detailed tests must be conducted to truly validate whether the algorithm meets the established requirements and effectively addresses the identified problems. Next, the source code should be made available, along with training sessions for the responsible team in order to transfer the necessary knowledge. In parallel, the process of implementing this change must be carefully examined, and the transition from the current practice to the new resolution method should be planned — taking into account the collection and processing of data required for running the algorithm. Once implemented, the focus should shift to keeping the system up to date through procedures that support the maintenance and continuous improvement of the algorithm, ensuring a meaningful and long-lasting transformation.

Appendix A

Optimization Model Implementation in Python-Gurobi

```
#!/usr/bin/env python3.11

# Copyright 2024, Gurobi Optimization, LLC

import gurobipy as gp
from gurobipy import GRB

import pandas as pd
import xlrd
from openpyxl import Workbook
from openpyxl import load_workbook

import time

# YOU MUST PUT sheet_name=None TO READ ALL SHEETS IN YOUR XLSM FILE
xlsm_file = "Modelo_Abdullah(2016)_v3 - Copia.xlsm"
df = pd.read_excel(xlsm_file, sheet_name='Planilha2', header=None)

# prints all sheets
# print(df)pip install xlrd

# Super Toy Problem

T=df.iloc[5,1]
J=df.iloc[2,1]
M = df.iloc[13,1]
```

```
A = df.iloc[12,1]
S = df.iloc[11,1]


C=[]
idx,idy = (17,1)
for t in range(T):
    temp = []
    for j in range(J):
        temp.append(df.iloc[idx+t,idy+j])
    C.append(temp)

N=[]
idx_n = 32
for t in range(T):
    temp1 = []
    idx_n = 32 + 11*t
    for h in range(J):
        temp2 = []
        for j in range(J):
            temp2.append(df.iloc[idx_n+h,1+j])
        temp1.append(temp2)
    N.append(temp1)

D=[]
for t in range(T):
    temp = []
    for j in range(J):
        temp.append(df.iloc[1+t,12+j])
    D.append(temp)


H=[]
for t in range(T):
    temp = []
    for j in range(J):
        temp.append(df.iloc[17+t,12+j])
    H.append(temp)

O=[]
idx_n = 32
for t in range(T):
    temp1 = []
    idx_n = 32 + 11*t
    for h in range(J):
        temp2 = []
        for j in range(J):
            temp2.append(df.iloc[idx_n+h,12+j])
        temp1.append(temp2)
```

```
    O.append(temp1)

C1=[]
idx,idy = (1,23)
for t in range(T):
    C1.append(df.iloc[idx+t,idy])

C2=[]
idx,idy = (17,23)
for t in range(T):
    temp = []
    for j in range(J):
        temp.append(df.iloc[idx+t,idy+j])
    C2.append(temp)

C3=[]
idx,idy = (32,23)
for t in range(T):
    temp = []
    for j in range(J):
        temp.append(df.iloc[idx+t,idy+j])
    C3.append(temp)


# Range of time and grade
time = range(T)
grade = range(J)

# Model

m = gp.Model("off-grade")
m.ModelSense = GRB.MINIMIZE

# Declare decison variables
x = m.addVars(grade, time, vtype=GRB.CONTINUOUS, name="(x)")
I = m.addVars(grade, time, vtype=GRB.CONTINUOUS, name="(I)")
y = m.addVars(grade, time, vtype=GRB.BINARY, name="(y)")
f = m.addVars(grade, time, vtype=GRB.BINARY, name="(f)")
z = m.addVars(time,grade,grade, vtype=GRB.BINARY, name="(z)")

sa = m.addVars(time, vtype=GRB.CONTINUOUS, name="(sa)")
aw = m.addVars(grade, time, vtype=GRB.CONTINUOUS, name="(aw)")
wc = m.addVars(grade, time, vtype=GRB.CONTINUOUS, name="(wc)")


# Using looping constructs, the preceding statement would be:
#
obj = sum(x[j,t]*C[t][j] for j in grade for t in time)
```

```
obj += sum(N[t][j][h]*O[t][j][h]*z[t,j,h] for j in grade for h in grade for t in time)
obj += sum(I[j,t]*H[t][j] for j in grade for t in time)
obj += sum(sa[t]*C1[t] for t in time)
obj += sum(aw[j,t]*C2[t][j] for j in grade for t in time)
obj += sum(wc[j,t]*C3[t][j] for j in grade for t in time)

m.setObjective(obj, GRB.MINIMIZE)

# Supplier Capacity Constraint
m.addConstrs((sa.sum(t) <= S for t in time), name="SupplierCapacityConstraint")

# Plant Capacity Constraint

constr1 = (x.sum(j,t) for j in range(J) for t in range(T))
# constr1 += (gp.quicksum(O[j] * z[t,j,h] for j in range(J) for h in range(J) for t in range(T)))
# constraints = m.addConstrs((gp.quicksum(x[j,t] for j in range(J) for t in range(T)) <= A for i in I), name="constraint")
m.addConstrs(((gp.quicksum(x[j,t] for j in range(J))) + (gp.quicksum(O[t][h][j] * z[t,j,h] for j in range(J) for h in range(J))) <= A for t in range(T)), name="AffiliateCapacityConstraint")

# Inventory Constraint
# m.addConstrs((x[j,t] + I[j,t-1] == aw[j,t] + I[j,t] for j in grade for t in range(1,T)), name="InventoryConstraint")

'''
Inventory Constraint alt
for t in range(T):
    if t == 0:
        m.addConstrs((x[j,t] == aw[j,t] + I[j,t] for j in grade), name="InventoryConstraint")
    else:
        m.addConstrs((x[j,t] + I[j,t-1] == aw[j,t] + I[j,t] for j in grade for t in range(1,T)), name="InventoryConstraint")
'''


# Inventory Constraint alt
for t in range(T):
    if t == 0:
        m.addConstrs((x[j,t] == aw[j,t] + I[j,t] for j in grade), name="InventoryConstraint")
    else:
        m.addConstrs((x[j,t] + I[j,t-1] == aw[j,t] + I[j,t] for j in grade), name="InventoryConstraint")
```

```
# Customer Demand
m.addConstrs((wc[j,t] == D[t][j] for j in grade for t in time), name="CustomerDemandConstraint")
# Transport Constraints
m.addConstrs((sa[t] == gp.quicksum(x[j,t] for j in range(J)) for t in time), name="TransportationConstraints")
# Warehouse inventory Constraints
m.addConstrs((aw.sum(j,t) - wc.sum(j,t) == 0 for j in grade for t in time), name="WarehouseInventoryConstraint")
# Sequencing Constraints
m.addConstrs((x[j,t] <= M*y[j,t] for j in grade for t in time), name="SequenceingConstraints (M)")
m.addConstrs((y[j,t] <= x[j,t] for j in grade for t in time), name="SequenceingConstraints (-)")
# Ensure fijt
for t in time:
    for j in range(J-1):
        LHS = y[j+1,t]
        for h in range(j+2,J):
            LHS += y[h,t]
        m.addConstr((LHS <= M*f[j,t]), name="Ensure_fijt (M)")
# Ensure fijt
for t in time:
    for j in range(J-1):
        LHS = y[j+1,t]
        for h in range(j+2,J):
            LHS += y[h,t]
        m.addConstr((LHS >= f[j,t]), name="Ensure_fijt (-)")
m.addConstrs((z[t,j,h] <= 0.5*(y[j,t] + y[h,t]) for j in range(J-1) for h in range(j+1,J) for t in time), name="Ensure1_zijht (0.5)")
m.addConstrs((gp.quicksum(z[t,j,h] for h in range(j+1,J)) >=  y[j,t] + f[j,t] - 1 for j in range(J-1) for t in time), name="Ensure2_zijht")
m.addConstrs((gp.quicksum(z[t,j,h] for j in range(h)) <=  1 for h in range(1,J) for t in time), name="Ensure3_zijht")
```

```
def printSolution():
    if m.status == GRB.OPTIMAL:
        print(f"\nZ: {m.ObjVal:g}")
        print("\nX:")
        for j in grade:
            for t in time:
                print(f"  X {x[j, t].X:g} Production of grade {j} @ month {t}")
        print("--------------------------------------")
        print("\nY:")
        for j in grade:
            for t in time:
                print(f"  Y {y[j, t].X:g} Allocation of grade {j} @ month {t}")
        print("--------------------------------------")
        print("\nI:")
        for j in grade:
            for t in time:
                print(f"  I {I[j, t].X:g} Inventory of grade {j} @ month {t}")
        print("--------------------------------------")
        print("\nf:")
        for j in grade:
            for t in time:
                print(f"  f {f[j, t].X:g} Produced of grade higher than {j} @ month {t}")
        print("--------------------------------------")
        print("\nz:")
        for j in grade:
            for h in grade:
                for t in time:
                    print(f"  z {z[t, j, h].X:g} Transitioned {j} to grade {h} @ month {t}")
    else:
        print("No solution")

def writeSolution():
    if m.status == GRB.OPTIMAL:


        wb = load_workbook(xlsm_file,keep_vba=True)
        ws = wb['Planilha2']

        idx,idy = (2,35)
        for j in grade:
            for t in time:
```

```
                ws.cell(row=idx+t,column=idy+j).value = x[j,t].X

        idx,idy = (18,35)
        for j in grade:
            for t in time:
                ws.cell(row=idx+t,column=idy+j).value = I[j,t].X

        idx,idy = (33,35)
        for j in grade:
            for t in time:
                ws.cell(row=idx+t,column=idy+j).value = y[j,t].X

        idx,idy = (54,35)
        for j in grade:
            for t in time:
                ws.cell(row=idx+t,column=idy+j).value = f[j,t].X

        idx,idy = (75,35)
        for t in time:
            idx = 75+11*t
            for j in grade:
                for h in grade:
                    ws.cell(row=idx+j,column=idy+h).value = z[t, j, h].X
                    # ws.cell(row=idx+j,column=idy+h).value = 999

        idx,idy = (2,46)
        for t in time:
            # ws.cell(row=idx+j,column=idy+t).value = z[j, h, t].X
            ws.cell(row=idx+t,column=idy).value = sa[t].X

        idx,idy = (18,46)
        for j in grade:
            for t in time:
                # ws.cell(row=idx+j,column=idy+t).value = z[j, h, t].X
                ws.cell(row=idx+t,column=idy+j).value = aw[j,t].X

        idx,idy = (33,46)
        for j in grade:
            for t in time:
                ws.cell(row=idx+t,column=idy+j).value = wc[j,t].X
                # ws.cell(row=idx+j,column=idy+t).value = 999

        wb.save(xlsm_file)


    else:
        print("No solution")
```

```

# Solve
m.write("model.lp")
m.optimize()
printSolution()
writeSolution()

print(m.Runtime)
```

content/Abdullah_2016–Copia.py

Bibliography

[1] Fortune Magazine. *Fortune Global 500 Rankings.* Accessed: 2024-03-10. 2024. URL: `https://fortune.com/ranking/global500/search/` (cit. on p. 1).

[2] Ahmed M. Ghaithan. «A Stochastic Programming Model for Production Planning and Sequencing of Multi-Grade Petrochemicals». In: *Proceedings of the 2nd African International Conference on Industrial Engineering and Operations Management.* King Fahd University of Petroleum & Minerals, Construction Engineering and Management Department, Dhahran, Saudi Arabia. Harare, Zimbabwe: IEOM Society International, 2020, pp. 1420–1429. URL: `https://www.ieomsociety.org` (cit. on pp. 1, 20).

[3] L.F.L. Moro, A.C. Zanin, and J.M. Pinto. «A Planning Model for Refinery Diesel Production». In: *Computers & Chemical Engineering* 23.8 (1999), pp. 1171–1188. DOI: `10.1016/S0098-1354(98)00209-9`. URL: `https://doi.org/10.1016/S0098-1354(98)00209-9` (cit. on p. 1).

[4] I. Bhieng Tjoa, Ramesh Raman, Toshiaki Itou, Kaoru Fujita, and Yukikazu Natori. «Impacts of Enterprise Wide Supply-Chain Management Techniques on Process Control». In: *Proceedings of the 1999 IEEE International Conference on Control Applications.* Kohala Coast-Island of Hawai'i, Hawai'i, USA: IEEE, 1999, pp. 605–608. DOI: `10.1109/CCA.1999.801140` (cit. on pp. 2, 20).

[5] Hesham K. Alfares. «A Mathematical Model for Optimum Petrochemical Multi-Grade Selection, Production, and Sequencing». In: *Proceedings of the Analysis of Manufacturing Systems (AMS 2007).* Presented at AMS 2007 Conference. King Fahd University of Petroleum & Minerals. Dhahran, Saudi Arabia, 2007, pp. 199–204 (cit. on pp. 2, 8, 20).

[6] David L. Cooke and Thomas R. Rohleder. «Inventory evaluation and product slate management in large-scale continuous process industries». In: *Journal of Operations Management* 24.3 (2006), pp. 235–249. DOI: `10.1016/j.jom.2004.08.009`. URL: `https://doi.org/10.1016/j.jom.2004.08.009` (cit. on pp. 3, 4, 11, 20).

[7] Mushabeb Z. Alqahtani, Arifusalam Shaikh, and Malick M. Ndiaye. «Focused Plant Optimization Strategy for Polyethylene Multi-Grades and Multi-Sites Production». In: *Arabian Journal for Science and Engineering* 43 (2018), pp. 3173–3185. DOI: 10.1007/s13369-017-2882-7. URL: https://doi.org/10.1007/s13369-017-2882-7 (cit. on pp. 4, 20, 32).

[8] Chia-Yen Lee, Chieh-Ying Ho, Yu-Hsin Hung, and Yu-Wen Deng. «Multi-objective genetic algorithm embedded with reinforcement learning for petrochemical melt-flow-index production scheduling». In: *Applied Soft Computing* 159 (2024), p. 111630. DOI: 10.1016/j.asoc.2024.111630. URL: https://www.elsevier.com/locate/asoc (cit. on p. 4).

[9] Felipe Machado Urban. «Modeling the Response to Unforeseen Events in Train Schedules». Supervised by Prof. Dr. Leonardo Junqueira. Graduation Thesis. São Paulo, Brazil: Escola Politécnica da Universidade de São Paulo, 2024. URL: https://github.com/Felipe-MU/Train-Rescheduling-Problem-TCC (cit. on p. 8).

[10] Michael Kupferschmid. *Introduction to Mathematical Programming: Theory and Algorithms of Linear and Nonlinear Optimization*. 1st. Licensed under CC-BY 4.0. Self-published, 2023. URL: https://creativecommons.org/licenses/by/4.0/legalcode.txt (cit. on p. 9).

[11] Wayne L. Winston. *Operations Research: Applications and Algorithms*. 4th. Belmont, CA, USA: Duxbury Press, 2003. ISBN: 9780534380588. URL: https://www.cengage.com (cit. on p. 9).

[12] Muhammad Rashid Ramzan, Nadia Nawaz, Ashfaq Ahmed, Muhammad Naeem, Muhammad Iqbal, and Alagan Anpalagan. «Multi-objective optimization for spectrum sharing in cognitive radio networks: A review». In: *Pervasive and Mobile Computing* 41 (2017), pp. 106–131. DOI: 10.1016/j.pmcj.2017.07.010. URL: https://doi.org/10.1016/j.pmcj.2017.07.010 (cit. on p. 9).

[13] George B. Dantzig. «Linear Programming». In: *Operations Research* 50.1 (2002), pp. 42–47. DOI: 10.1287/opre.50.1.42.17798. URL: https://doi.org/10.1287/opre.50.1.42.17798 (cit. on p. 9).

[14] Mehdi Mrad and Hesham K. Alfares. «Optimum Multi-Period, Multi-Plant, and Multi-Supplier Production Planning for Multi-Grade Petrochemicals». In: *International Journal of Industrial Engineering: Theory, Applications and Practice* 23.6 (2016), pp. 399–411. ISSN: 1943-670X. URL: https://www.researchgate.net/publication/313915450 (cit. on pp. 9–11).

[15] T. Castillo-Calzadilla, M.A. Cuesta, Carlos Quesada, C. Olivares-Rodriguez, M. Macarulla, J. Legarda, and C.E. Borges. «Is a massive deployment of renewable-based low voltage direct current microgrids feasible? Converters, protections, controllers, and social approach». In: *Energy Reports* 8 (2022), pp. 12302–12326. DOI: 10.1016/j.egyr.2022.09.067. URL: https://doi.org/10.1016/j.egyr.2022.09.067 (cit. on p. 9).

[16] Ludo F. Gelders and Luk N. Van Wassenhove. «Production Planning: A Review». In: *European Journal of Operational Research* 7.2 (1981), pp. 101–110. DOI: 10.1016/0377-2217(81)90271-X (cit. on pp. 10, 13).

[17] Alex J. Ruiz-Torres and Farzad Mahmoodi. «Analysis of Multi-Cell Production Systems Considering Cell Size and Worker Flexibility». In: *International Journal of Industrial Engineering* 15.4 (2008). Received 15 June 2007; Accepted in revised form 4 February 2008, pp. 360–372. ISSN: 1072-4761. URL: https://www.ijie.org (cit. on p. 11).

[18] R.L. Tousain and O.H. Bosgra. «Market-oriented scheduling and economic optimization of continuous multi-grade chemical processes». In: *Journal of Process Control* 16.3 (2006), pp. 291–302. DOI: 10.1016/j.jprocont.2005.06.009. URL: https://www.elsevier.com/locate/jprocont (cit. on pp. 11, 12, 17).

[19] Billy Rigby, Leon S. Lasdon, and Allan D. Waren. «The Evolution of Texaco's Blending Systems: From OMEGA to StarBlend». In: *Interfaces* 25.5 (1995), pp. 64–83. DOI: 10.1287/inte.25.5.64. URL: http://dx.doi.org/10.1287/inte.25.5.64 (cit. on p. 11).

[20] Kenneth R. Baker and Dan Trietsch. *Principles of Sequencing and Scheduling.* 2nd. Wiley Series in Operations Research and Management Science. Originally published in 2009 (1st edition). Hoboken, NJ, USA: John Wiley & Sons, 2019. ISBN: 9781119262589. URL: https://www.wiley.com (cit. on pp. 11, 12).

[21] B. Karimi, S.M.T. Fatemi Ghomia, and J.M. Wilson. «The Capacitated Lot Sizing Problem: A Review of Models and Algorithms». In: *Omega* 31.5 (2003), pp. 365–378. DOI: 10.1016/S0305-0483(03)00059-8 (cit. on pp. 13, 14).

[22] Sari Abdullah, Abdulrahim Shamayleh, and Malick Ndiaye. «Capacitated Lot-Sizing and Scheduling with Sequence-Dependent Setups in Petrochemical Plants». In: *Proceedings of the 2016 International Conference on Industrial Engineering and Operations Management.* Available at: https://www.ieomsociety.org/kl2016/proceedings.pdf. IEOM Society International. Kuala Lumpur, Malaysia, Mar. 2016, pp. 1835–1843 (cit. on pp. 17, 19, 20, 48).

[23] Hesham K. Alfares. «Optimum multi-plant multi-supplier production planning for multi-grade petrochemicals». In: *Engineering Optimization* 00.0 (2009), pp. 1–10. DOI: 10.1080/03052150802596084 (cit. on p. 20).

[24] M. Joly, L. F. L. Moro, and J. M. Pinto. «Planning and Scheduling for Petroleum Refineries Using Mathematical Programming». In: *Brazilian Journal of Chemical Engineering* 19.2 (2002), pp. 207–228. DOI: 10.1590/S0104-66322002000200008. URL: https://www.scielo.br/j/bjce/a/yDJgLjWLSvcyVpMp5cCRXKv/abstract/?lang=en (cit. on p. 20).

[25] Karen V. Pontes, Inga J. Wolf, Marcelo Embiruçú, and Wolfgang Marquardt. «Dynamic Real-Time Optimization of Industrial Polymerization Processes with Fast Dynamics». In: *Industrial & Engineering Chemistry Research* 54.46 (2015), pp. 11881–11893. DOI: 10.1021/acs.iecr.5b00909. URL: https://doi.org/10.1021/acs.iecr.5b00909 (cit. on p. 20).

[26] Adrian Prata, Jan Oldenburg, Andreas Kroll, and Wolfgang Marquardt. «Integrated Scheduling and Dynamic Optimization of Grade Transitions for a Continuous Polymerization Reactor». In: *Computers and Chemical Engineering* 32.2 (2008), pp. 463–476. DOI: 10.1016/j.compchemeng.2007.03.009. URL: https://doi.org/10.1016/j.compchemeng.2007.03.009 (cit. on p. 20).

[27] Shangyi Yang, Chao Sun, and Youngok Kim. «Indoor 3D Localization Scheme Based on BLE Signal Fingerprinting and 1D Convolutional Neural Network». In: *Electronics* 10.15 (2021), p. 1758. DOI: 10.3390/electronics10151758. URL: https://www.mdpi.com/2079-9292/10/15/1758 (cit. on p. 27).

[28] Microsoft Corporation. *Visual Studio and Visual Studio Code*. Accessed: 2024-03-10. 2024. URL: https://visualstudio.microsoft.com/pt-br/#vscode-section (cit. on p. 29).

[29] Python Software Foundation. *Tutorial — Python 3 Documentation (Portuguese)*. Accessed: 2024-03-10. 2024. URL: https://docs.python.org/pt-br/3/tutorial/index.html (cit. on p. 29).

[30] The pandas development team. *pandas: Python Data Analysis Library*. Accessed: 2024-03-10. 2024. URL: https://pandas.pydata.org/ (cit. on p. 30).

[31] Gurobi Optimization, LLC. *Gurobi Optimizer*. Accessed: 2024-03-10. 2024. URL: https://www.gurobi.com/solutions/gurobi-optimizer/ (cit. on p. 30).

[32] VivaReal. *Aluguel de Galpões Comerciais em Mauá, SP*. Accessed: 2024-03-10. 2024. URL: https://www.vivareal.com.br/aluguel/sp/maua/galpao_comercial/?transacao=aluguel&onde=,S%C3%A3o%20Paulo,Mau%C3%A1,,,,,city,BR%3ESao%20Paulo%3ENULL%3EMaua,-23.666558,-46.459915,&tipos=galpao_comercial&pagina=1 (cit. on p. 34).

[33] GoFretes. *GoFretes: Plataforma de Cotações de Frete*. Accessed: 2024-03-10. 2024. URL: https://gofretes.com.br/ (cit. on p. 34).