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## Abstract

In this prospective paper, we sought to theoretically assess the magnitude order of the benefits related to an in-depth analysis of a high-profile decision-making problem of the oil industry. A simplified representation of the crude oil allocation planning problem in the State of São Paulo is focused on. The scope of the problem comprises 4 oil refineries, which are responsible for approximately one-half of the current Brazilian refining capacity, more than 260 crude oil types and 5 key properties of interest for primary processing in crude distillation units (CDUs). The optimization criterion was economic and considered the crude oil pricing, pumping costs through long crude oil pipelines, and the incomes from intermediary cuts in CDUs. Real-world data, whenever available, were used to run the computation experiments. The major finding of this study shows that, depending on the problem instance considered, the planning model based on monthly time discretization can overestimate the profitability of the entire system by less than 1%, on average, in relation to its weekly discretized representation, the so-called "plannuling" model.

## 1 Introduction

The increased efficiency of modern computer technologies allied to the development of powerful optimization algorithms ( KARMAKAR, 1984; VISWANATHAN ; GROSSMANN, 1990; DRUD, 1996; IBM, 2012) for solving large-scale decision-making problems have amplified the possibilities of mathematical modeling approaches (KELLY , FORBES, 1998; KONDILI et al., 1993; PANTELIDES, 1994) in an unprecedented way. In this context, Operational Research (OR)<sup>1</sup> techniques (HILLIER; LIEBERMAN, 2005) and large-scale optimization (BIEGLER; GROSSMANN, 2004; GROSSMANN ; BIEGLER, 2004) have proven to be instrumental to achieve important progress in many fields of science and technology, with innovative solutions being successfully implemented on myriad real-world optimization problems (CUTHRELL and BIEGLER, 1987; NEIRO ;PINTO, 2004; JOLY; PINTO, 2006).

The application of OR techniques in the oil industry may be posed as an illustrative example. Right after the initial forays in linear programming, late in the 1940s, Dantzig (1949), Charnes; Cooper, and Mellon (1952) and Sysmonds (1955) were among the first in applying mathematical programming techniques to this business, thereby rendering the oil industry the first target of industrial applications of OR following its pioneer use in World War II. Since then, an enormous advancement of algorithms and modeling techniques to solve complex, real-world decision-making problems has unsurprisingly been produced in tight collaboration with or led by an illustrious set of chemical engineers (IGNÁCIO E. GROSSMANN; LORENTZ T. BIEGLER, among many others unintentionally left out).

Besides the largest, the oil sector is indeed a conspicuous example of the most complex chemical industries, involving many different and complex processes with numerous logistic connections among their elements. Usually, the common objective of petroleum refineries is to minimize the plant operational cost in harmony with macroscopic (tactical) economic guidelines optimally determined at the refinery planning level. In this kind of business, acting under certainty is of paramount importance; product quality must be met through safe plant operation. In general, such eminent goals are achieved through the integrated, optimal management of available resources at both local (LEE et al., 1996; JOLY et al., 2001) and corporate levels (NEIRO ; PINTO, 2004).

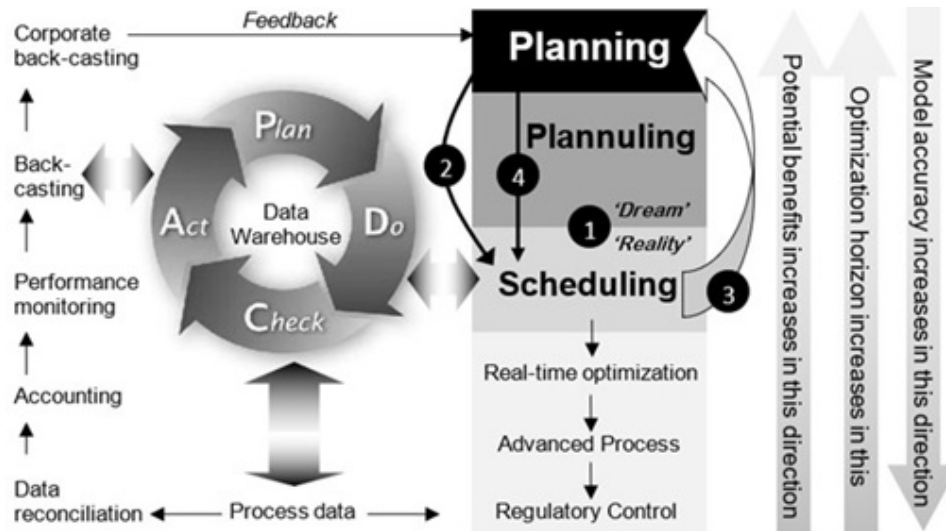
Undoubtedly, intelligent production planning and scheduling are currently of supreme importance to ensure refinery profitability, logistic reliability and safety at the local and corporate levels (JOLY, 2012). In Brazil, such activities play a particularly critical role, since the Brazilian downstream model is moving towards a demand-driven model rather than a supply-driven one. Moreover, new and specialized non-linear constraints are continuously being incorporated into these large-scale problems. Here, one can mention increases in oil prices implying the need for processing poor quality crudes, increasing demand and new demand patterns for petroleum products, new stringent environmental regulations related to clean fuels and start-up of new production technologies embedded into more complex refining schemes based on novel business models ( in-line certification units (FEITAL et al., 2013)).

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<sup>1</sup> *Abbreviations used in this paper:* CDU, crude distillation unit; LP, linear programming; NLP, nonlinear programming; OR, Operations Research.

Historically, this has been successfully, but not always optimally, achieved by exploiting decomposition approaches (Figure 1), instead of tackling the comprehensive large-scale optimization problem at once (SHAH et al, 2010).

Figure 1 - Conceptual model of a hierarchical decision-making structure for solving complex supply-chain problems in the oil industry.



Source: elaborated by the authors.

Whereas production planning is the business layer in which one should 'dream' in order to make more money (1), money loss minimization is what should be pursued through an optimal (i.e., 'planning-adherent') production scheduling in real-world settings. Given that production scheduling not only translates strategic objectives into operational actions (2) but also provides a valuable bridge for model maintenance and sophistication (3), we argue that additional efforts must be devoted to qualitatively and quantitatively improve the planning guidelines. In particular, we argue that one should explore the gap between strategic planning and operational scheduling by proposing a new tactical business layer here named 'plannuling', a term coined from the merge of words planning and scheduling.

By considering a more detailed representation of the planning model, this new intermediary layer is aimed to provide more guidelines which must be satisfied at the production scheduling level. In other words, the plannuling model aims to improve the adherence between the strategic and the operational worlds. As the planning model, the plannuling model should also consider a reasonable trade-off between complexity and computational expense, that is, it should ideally be tractable through optimization in order to provide marginal information. This information, which is the true link between two adjacent business layers in a hierarchical planning structure such as the one here proposed, should drive the search for a good solution at the production scheduling layer.

In many cases, prior solutions were also focused on the independent analyses of specific parts of the petroleum supply chain, often leading to a lack of integration of the whole problem ( LEE et al., 1996; PINTO et al., 2000; JOLY ;PINTO, 2003).

In the past few decades, however, the full integration in the oil supply chain was in evidence. From a contextual perspective, one has the economy globalization which has established new competition patterns. Furthermore, globalization trends have significantly increased the scale and complexity of the modern enterprise. The enterprise has been transformed into a global network consisting of multiple business units and functions (VARMA et al., 2007). From a practical standpoint, the computational treatment (GAREY ; JOHNSON, 1979) of this challenging class of engineering problems in OR and management sciences has increasingly become feasible. In the light of advanced technologies developed over the past two decades, we have really witnessed a robust increase of published works addressing the intelligent management of supply-chain systems or subsystems (MAGALHÃES, 2004; LASSCHUIT ; THIJSSSEN, 2004; PINTO ; NEIRO, 2004). Whereas production planning has received major attention by the OR community since the 1950s up to the 1990s, the study of production scheduling became an important focus of investigation since then underscored by the facilities introduced by high-level languages, user-friendly modeling systems ( GAMS, AIMMS, etc.). In this prolific context for novel applied developments, the short-term production scheduling of crude oil and oil products of real-world oil refineries has largely been investigated ( LEE et al., 1996; JOLY ; PINTO, 2003; MONIZ et al., 2013; KELLY et al., 2006).

However, the search for efficient modeling frameworks able to minimize the gap between production planning and scheduling is an aspect to be further investigated. In this vein, Rocha et al. (2009) worked on the gap between the strategic and operational levels at Brazilian supply chain, a subject masterly reviewed by Iachan (2009) who summarized the major Brazilian in-house developments in the exciting field of OR over the past 40 years. In the Brazilian oil sector, there are many notorious corporate-wide OR projects aimed to improve the operation performance. Here are included optimization of fleet sizing and routing for off-shore operations, sophisticated LP-based models for solving the Brazilian oil industry supply-chain, advanced (and visionary) refinery scheduling systems (MAGALHÃES et al., 1998; JOLY, 2012), specialized applications for real-time optimization (COSTA et al., 2008), and advanced process control applications (MORO ; GROSSMANN, 2013).

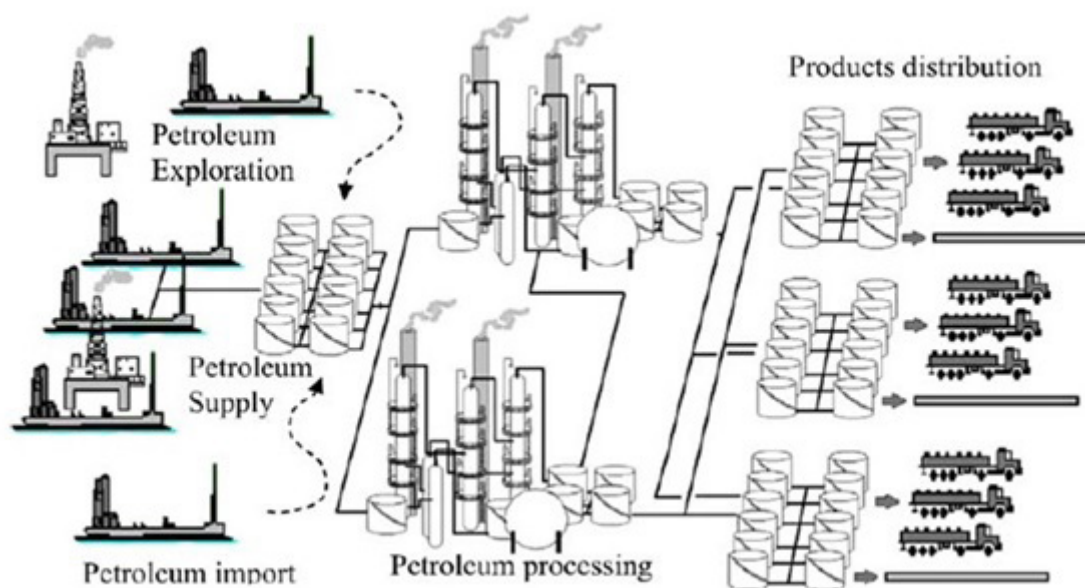
Despite undeniable recent advances, the petroleum allocation activity remains an extraordinary challenge. As illustrated in **Figure 2**, Petroleum exploration is at the highest level of the chain (left). At the strategic level, decisions regarding petroleum exploration include design and planning of oil field infrastructure. Operationally, petroleum may be also supplied from international sources. Oil vessels transport petroleum to maritime terminals, which are connected to other terminals or refineries through a pipeline network. Decisions at this level incorporate transportation modes and supply planning and scheduling, the subject addressed in this work. Crude oil is converted into products in refineries; the latter can be connected to each other in order to take advantage of each refinery design within the complex.

This is the case of the São Paulo area, which comprises 4 refineries logistically interconnected by a complex pipeline network. Oil products generated at the refineries are then sent to distribution centers. Crude oil and products up to this level are often transported through pipelines. From this level on, products can be transported through different modes (e.g., pipelines, vessels, trains or trucks) depending on distances, product type or consumer demands. In general, production planning includes decisions

such as individual production levels for each product as well as operating conditions for each refinery in the network, whereas product transportation focuses on scheduling and inventory management of the distribution network.

The complex organizational structures underlying horizontally and vertically integrated chemical process industries, such as the oil sector, challenge our understanding of cross-functional co-ordination and its business impact (VARMA et al., 2007). In this particular case, petroleum allocation may be considered a critical link for integrating the petroleum supply chain of many oil companies, such as Petrobras (discussed in ROCHA et al., 2009) or Shell (LASSCHUIT; THIJSSSEN, 2004). Representing a large-scale system with a high combinatorial aspect and important nonlinearities involved, the problem has continuously been a major focus of interest of bright chemical (or, more generally, process) engineers and OR analysts with open minds to test new tools and to find new solutions.

Figure 2 - A general schematic representation of the oil industry supply chain.



Source: Neiro and Pinto (2004).

Undeniably, we are dealing with a complex system (OTTINO, 2003). Consequently, since a large number of simplifications are unavoidably needed, this may lead to suboptimal operation due to differences between modeling approaches (planning vs. scheduling) and loss of information throughout the hierarchical structure (Figure 1). As the time horizon of interest is usually smaller when operational decisions must be scheduled, the number of details to be considered becomes higher and, therefore, a proper representation of the operational (scheduling) problem will have more variables and constraints than the planning model typically does.

As a consequence, the planning model normally provides different (i.e., not 'implementable') optimal solutions than ones that are effectively implemented. In particular, as some constraints (e.g., operational constraints) need to be disregarded at the highest levels, the top-down flow of information throughout the supply chain model may be not complete or accurate, thereby introducing additional degrees of freedom or inaccuracies to be resolved at the lowest levels.

In this sense, reducing the gap between strategic and operational decisions may represent a prolific way for achieving improvements in the integrated management of complex supply chains. Current advances in IT and algorithms enable (and motivate) modelers to sophisticate planning models thereby minimizing the aforementioned problems which are mostly due to distinct representations of the same problem. As discussed in Figure 1, one candidate approach is to propose a new, intermediary business layer between planning and scheduling, which we name *plannuling* (the merge between planning and scheduling). This new layer is devoted to address the planning problem but also regarding representative scheduling constraints, such as time-dependent resources (in this case, the dynamic availability of crude oil at its source).

At this point, a key question arises: how may such a sophisticated (i.e., detailed) modeling approach contribute to improving the operational decisions? To the best of our knowledge, there is no published information about the solution quality gap between a 'conventional' (i.e., time-aggregated) and a detailed (i.e., in which the planning horizon is discretized in accordance with master time events taken into account for scheduling decisions) planning model.

This paper aims to theoretically quantify this gap based on comparisons between planning and *plannuling* models, in which differences in the modeling approach are restricted to time representation. Specifically, we address the real-world problem of crude oil allocation in São Paulo State (Brazil), where 4 oil refineries respond to approximately one-half of the Brazilian refining capacity.

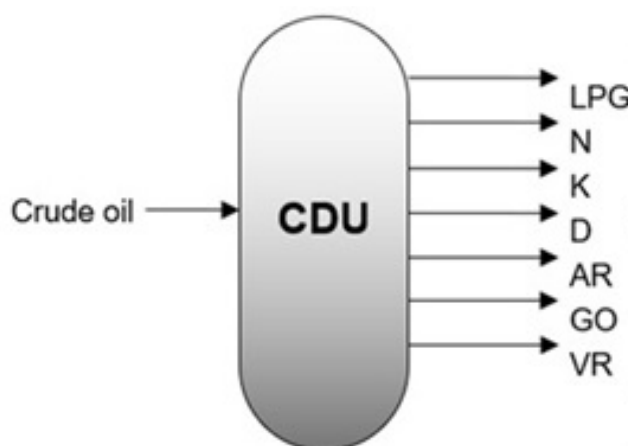
This article is structured as follows. Problem definition is stated in Section 2 whereas Section 3 is devoted to present the proposed modeling formulations and rationales. The solution method is described in Section 4. *In silico* results are summarized in Section 5 and discussed in Section 6. Lastly, Section 7 concludes the paper and outlines future research.

## 2 Problem definition

The crude oil supply chain in the State of São Paulo comprises one maritime terminal and four interconnected oil refineries (REFINERY A to REFINERY D). Given a monthly forecast related to the potential availability of 263 crude types in the maritime terminal, the problem we are concerned with is to determine the optimal allocation between the available quantity of each type of crude oil and each refinery.

In this study, we hypothesize that each refinery has a single petroleum distillation unit (CDU), which represents, in a simplified way, the actual hardware configuration of each refinery's distillation process. This simplified representation also admits a unified CDU model for the existing atmospheric and vacuum distillations in the refinery, as schematically represented in Figure 3.

Figure 3 - Simplified representation of the crude distillation process.



Source: elaborated by the authors.

According to this model, crude oils are fractionated into liquefied petroleum gas (LPG), naphtha (N), kerosene (K), diesel (D) and "bottom cuts". These can be either atmospheric residue (AR) or gasoil (GO) plus vacuum residue (VR).

The first case (the bottom cut is AR) corresponds to the case of REFINERY A, which is equipped with a residue fluid catalytic cracking (RFCC) unit. In this case, GO + VR yield is set to zero. The second situation (bottom cuts are GO and VR) is valid for REFINERY B, REFINERY C and REFINERY D, whose refining schemes are based on conventional fluid catalytic cracking (FCC) units. In this case, the AR yield is set to zero.

Here, we consider that each CDU can produce at most 6 intermediary streams (or cuts), namely: liquefied petroleum gas (LPG), naphtha (N), kerosene (K), diesel (D) and "bottom cuts" which can either be Atmospheric residue (AR) or Gasoil (GO) and vacuum residue (VR).

Four physical-chemical properties (or qualities) are managed in the model. They are crude API, crude acidity, carbon residue related to the heavier cut (RAT or AR and density. The latter is required in order to calculate blending rules on a mass basis.

At the beginning of the one-month planning horizon, the crude oil availability in the maritime terminal is known in terms of crude types and their corresponding initial volumes. Crudes are characterized by: a) a constant yield profile for processing in CDUs, and b) fixed qualities (crude API and crude acidity).

The crude quality set of interest is completed by the carbon residue in the CDU bottom cut. This process stream may correspond to an atmospheric residue (AR) for further processing into a residue fluid

catalytic cracking (RFCC) unit in REFINERY A refinery or a vacuum residue (VR) for further processing in delayed coker units in the remaining refineries (REFINERY C, REFINERY D ; REFINERY B).

Each refinery is characterized by a particular set of constraints. These constraints are categorized into two classes:

- mass balance constraints: the optimal allocation of crude oil must satisfy lower and upper bounds of processing loads in each refinery. Also, the volumetric yield of certain CDU cuts is bounded;
- quality constraints: the optimal allocation of crude oil must satisfy lower and/or upper bounds of the blend mix quality. The quality of certain CDU cuts is also subject to specification constraints.

The optimization criterion is economic. Operational costs are represented by raw material (crude oils in the maritime terminal) and pumping costs throughout the oil pipelines. Operational revenues are due to the production of intermediary cuts in CDUs.

### 3 Mathematical modeling

The following are the assumptions for the nonlinear programming (NLP) based models that are proposed herein:

(a1) the initial system conditions are known a priori;

(a2) the system is isothermal and at ambient temperature;

(a3) all intermediate and final products are incompressible fluids. In addition, due to the lack of chemical reactions, there is no volumetric expansion or reduction in CDUs or blending operations;

(a4) aggregated storage capacity at each site (i.e., at the maritime terminal and at each oil refinery). Moreover, we neglect the crude oil inventories inside oil pipelines by assuming instantaneous transportation;

(a5) transportation times and product mixing inside oil pipelines are neglected. In a similar way, since discrete operations (e.g., resource selection and sequencing) are not taken into account, changeover times are neglected.

Assumption (a1) defines the optimization model instance. Assumption (a2) is essential to simplify the model since there are large temperature differences between processing units and pipelines or storage tanks. Assumption (a3) guarantees that neither thermal contraction nor expansion of the molar volume occurs in blending operations or processing in CDUs, which is relevant since the model relies on volumetric calculations. Lastly, assumptions (a4) are stated in benefit of a simpler (i.e., continuous) mixed-integer formulation: whereas refineries are complex systems which need to be fed by proper amounts and types of crudes in order to supply their market with the required products, operational details of refinery operation modeling were omitted or simplified in this study.

Each optimization model presented herein yields an NLP which is composed of an objective function (Eq. 1) and constraints (Eq. 1-10) according to nomenclature defined in Table 1. In what follows, each model constraint is presented in both representations proposed. The planning model, which considers the whole month as a single time period, is identified by an additional letter 'a' in the equation number (e.g., 1a, 2a, and so on), whereas identifier 'b' (e.g., 1b, 2b, and so on) refers to the planning model in which the whole month is uniformly discretized in 4 weeks.

Table 1 - Model nomenclature.

Indices and Sets	Description
$c$	CDU cuts
$p$	Crude oil types
$r$	Refineries
$w$	Weeks
Parameters	Description
$nd$	Number of days considered in the time horizon
$ACD_p$	Acidity for crude oil $p$
$ACD_r^{max}$	Upper bound for acidity of the crude oil mix in refinery $r$
$API_p$	API for crude oil $p$
$API_r^{max}$	Upper bound for API of the crude oil mix in refinery $r$
$API_r^{min}$	Lower bound for API of the crude oil mix in refinery $r$
$Cost_p^{oil}$	Crude oil $p$ price at maritime terminal
$Cost_{p,r}^{CorPump}$	Pumping cost of oil $p$ to refinery $r$
$V_{c,r}^{maxcut}$	Maximum capacity of intermediary cut $c$ in refinery $r$ ( $c$ = naphtha, kerosene, diesel, RAT)
$RES_{p,r}^{min}$	RCR/RCC content for RAT/RV from crude oil $p$ in refinery $r$
$RES_r^{min}$	Lower bound for RCR/RCC in the RAT from crude oil mix in refinery $r$
$RES_r^{max}$	Upper bound for RCR/RCC in the RAT from crude oil mix in refinery $r$
$revcut_{c,r}$	Revenue price for each cut $c$ in refinery $r$
$P_p$	Density for crude oil $p$
$VD_r^{min}$	Minimum volumetric demand of crude oil in refinery $r$ per day
$VD_r^{max}$	Maximum volumetric demand of crude oil in refinery $r$ per day
$V_0$	Initial volume of crude oil at maritime terminal (received) in the month under consideration
$V_{0,p,w}$	Initial volume of crude oil at maritime terminal (received) during the week $w$ under consideration
$assay_{c,p}$	Volumetric yield for intermediary cut $c$ with respect to crude $p$ at refinery $r$
Variables	Description
$ACD^{aloc}$	Acidity of the allocated crude oil mix in refinery $r$ during the month under consideration
$ACD_{r,w}^{aloc}$	Acidity of the allocated crude oil mix in refinery $r$ during the week $w$ under consideration
$API_r^{aloc}$	API of the allocated crude oil mix in refinery $r$ during the month under consideration
$API_{r,w}^{aloc}$	API of the allocated crude oil mix in refinery $r$ during the week $w$ under consideration
$VD_{p,r}$	Overall quantity of crude oil $p$ from maritime terminal to refinery $r$ during the month under consideration
$VD_{p,r,w}^{aloc}$	Overall quantity of crude oil $p$ from maritime terminal to refinery $r$ during the week $w$ under consideration
Variables	Description
$product_{c,r}$	Intermediary cuts $c$ of crude oil $p$ production in refinery $r$ during the month under consideration
$product_{c,r,w}$	Cuts $c$ of crude oil $p$ production in refinery $r$ during the week $w$ under consideration
$profit$	Profit calculation
$RES_r^{aloc}$	RCR/RCC in the RAT from the allocated crude oil mix in refinery $r$ during the month under consideration
$RES_{r,w}^{aloc}$	RCR/RCC in the RAT from the allocated crude oil mix in refinery $r$ during the week $w$ under consideration
$Stock\ level_{p,w}$	The amount of crude oil received in the week added to the amount that was not allocated from the week before

Source: elaborated by the authors.

The objective function.

Maximize profit, where:

Profit = Receipt from intermediary cuts – inventory cost – pumping cost.

Or, mathematically:

$$\begin{aligned}
 \text{profit} = & \sum_{c=1}^c \sum_{r=1}^r \text{product}_{c,r} \cdot \text{revcut}_{c,r} + \\
 & - \sum_{p=1}^p \text{cost}^{\text{oil}}_p \cdot \text{VD}_{p,r}^{\text{aloc}} - \sum_{p=1}^p \sum_{r=1}^r \text{Cost}_{p,r}^{\text{CorPump}} \cdot \text{VD}_{p,r}^{\text{aloc}} \quad (1a)
 \end{aligned}$$

$$\begin{aligned}
 \text{profit} = & \sum_{c=1}^c \sum_{r=1}^r \sum_{w=1}^w \text{product}_{c,r,w} \cdot \text{revcut}_{c,r} + \\
 & - \sum_{p=1}^p \sum_{w=1}^w \text{cost}^{\text{oil}}_p \cdot \text{VD}_{p,r,w}^{\text{aloc}} + \\
 & - \sum_{p=1}^p \sum_{r=1}^r \sum_{w=1}^w \text{cost}_{p,r}^{\text{CorPump}} \cdot \text{VD}_{p,r,w}^{\text{aloc}} \quad (1b)
 \end{aligned}$$

### The crude oil supply constraints

The total amount of crude oil received through oil-pipelines must meet the foreseen demand defined at the corporate planning.

$$\text{VD}_r^{\text{Min}} \leq \text{VD}_{p,r}^{\text{aloc}} \leq \text{VD}_r^{\text{Max}} \quad (2a)$$

$$\text{VD}_r^{\text{Min}} \leq \text{VD}_{p,r,w}^{\text{aloc}} \leq \text{VD}_r^{\text{Max}} \quad (2b)$$

The total amount of crude oil sent by oil-pipelines during the month must consider the availability of the crude oil in the maritime terminal. In the planning analysis, however, the availability of crude oil in the maritime terminal at the beginning of the second, third and fourth weeks will correspond to the remaining inventory from the previous week (i.e., the amount that was not allocated) plus the amount of crude oil received from crude oil vessels that week.

$$\text{VD}_{p,r}^{\text{aloc}} \leq V_0 \quad (3a)$$

$$\begin{aligned}
 \text{VD}_{p,r,w}^{\text{aloc}} & \leq \text{Stock level}_{p,w} = \\
 & = V_{0p,w} + (\text{Stock level}_{0p,w-1} - \text{VD}_{p,r,w-1}^{\text{aloc}}) \quad (3b)
 \end{aligned}$$

### The production constraints

The production of intermediary cuts of atmospheric distillation must meet the processing in each refinery and its maximum supported capacity.

$$product_{c,r} = \sum_{p=1}^p c_{p,r} \cdot VD_{p,r}^{aloc} \leq V_{c,r}^{maxcut} \quad (4a)$$

$$product_{c,r,w} = \sum_{p=1}^p c_{p,r,w} \cdot VD_{p,r}^{aloc} \leq V_{c,r}^{maxcut} \quad (4b)$$

### The API constraints

The API of the crude oil blend mix sent through oil-pipelines is calculated using mixing rules on a mass basis and it must obey processing constraints at each refinery.

$$API_r^{min} \leq API_r^{aloc} \leq API_r^{max} \quad (5a)$$

$$API_r^{min} \leq API_{r,w}^{aloc} \leq API_r^{max} \quad (5b)$$

$$API_r^{min} = \frac{\sum_{p=1}^p (VD_{p,r}^{aloc} \cdot \rho_p \cdot API_p)}{\sum_{p=1}^p (VD_{p,r}^{aloc} \cdot \rho_p)} \quad (6a)$$

$$API_r^{min} = \frac{\sum_{p=1}^p (VD_{p,r,w}^{aloc} \cdot \rho_p \cdot API_p)}{\sum_{p=1}^p (VD_{p,r,w}^{aloc} \cdot \rho_p)} \quad (6b)$$

### The acidity constraints

Similarly, the acidity of the crude oil blend mix sent through oil-pipelines is calculated using mixing rules on a mass basis and it must obey processing constraints at each refinery.

$$ACD_r^{aloc} \leq ACD_r^{max} \quad (7a)$$

$$ACD_{r,w}^{aloc} \leq ACD_r^{max} \quad (7b)$$

$$API_r^{aloc} = \frac{\sum_{p=1}^p (VD_{p,r}^{aloc} \cdot \rho_p \cdot ACD_p)}{\sum_{p=1}^p (VD_{p,r}^{aloc} \cdot \rho_p)} \quad (8a)$$

$$ACD_{r,w}^{aloc} = \frac{\sum_{p=1}^p (VD_{p,r,w}^{aloc} \cdot \rho_p \cdot ACD_p)}{\sum_{p=1}^p (VD_{p,r,w}^{aloc} \cdot \rho_p)} \quad (8b)$$

### The RCR constraints

The content of carbon residue in the CDU bottom cut is also determined using mixing rules on a mass basis and it must obey processing constraints at each refinery.

$$RES_r^{min} \leq RES_r^{aloc} \leq RES_r^{max} \quad (9a)$$

$$RES_r^{min} \leq RES_{r,w}^{aloc} \leq RES_r^{max} \quad (9b)$$

$$RES_r^{aloc} = \frac{\sum_{p=1}^p (VD_{p,r}^{aloc} \cdot p_p \cdot RES_{p,r})}{\sum_{p=1}^p (VD_{p,r}^{aloc} \cdot p_p)} \quad (10a)$$

$$RES_{r,w}^{aloc} = \frac{\sum_{p=1}^p (VD_{p,r,w}^{aloc} \cdot p_p \cdot RES_{p,r})}{\sum_{p=1}^p (VD_{p,r,w}^{aloc} \cdot p_p)} \quad (10b)$$

## 4 Solution algorithm

It is worth noting that the major difficulty of this problem is due to bilinear terms in the mathematical model, which arise from the product between two variables. As a result, the model is non-convex (LEE et al., 1996). Therefore, a global optimal solution cannot be ensured. Most importantly, when trying to solve the NLP model as is, we found severe numerical difficulties regarding model initialization.

In fact, this was not surprising since NLP-based optimization problems may require a good initial solution. To overcome this difficulty, we proposed a bi-level solution framework in which an initial point was determined through running a linear programming (LP) based model, which is derived from the NLP model and is composed only by the linear constraints of the NLP model. Once this initial guess was determined and considered as the starting point for the NLP optimization, the full model was successfully solved in acceptable CPU times.

## 5 Results and discussion

The model modeling system GAMS was used to implement the model and its solution method. Computational experiments were based on fictitious, nevertheless realistic data and performed on an IntelCore i7 2.0 GHz 2.0 GB RAM. When solving the LP and NLP models, we tested different solvers in order to assess the objective function value variation, which was around 0.35%. This reduced variation showed that the solution quality is not significantly affected by solver selection. Overall, at most

0.61 CPU seconds was required to solve an instance the optimization problem. Table 2 summarizes dimensional aspects of both models.

Table 2 - Model statistics for a one-month horizon.

	Planning		Plannuling	
	LP	NLP	LP	NLP
Blocks of equations	9	17	11	19
Single equations	86	112	2022	2126
Blocks of variables	3	6	4	7
Single variables	161	171	5293	5333
Non-zero elements	1308	1664	45520	55944

Source: elaborated by the authors.

Computational experiments considered 12 fictitious, nevertheless realistic instances of the problem for 6 months (M1 to M6). In particular, 06 instances were related to the aggregated analysis of the problem (the planning model) whereas the remaining 6 ones considered each month discretized into 4 periods (the plannuling model). Economic parameters, which include the raw-material cost as well as the internal revenue price for each cut at each refinery and pumping costs, are described in Tables 3 and 4 whereas major bounds on operational and processing variables are summarized in Table 5.

Table 3 - Internal revenue price (US\$/m<sup>3</sup>).

Cut	REFINERY			
	A	B	C	D
LGP	174	174	188	226
N	345	349	346	346
K	438	435	454	471
D	438	435	455	452
AR	263	0	0	0
GO	0	380	380	380
VR	0	260	240	252

Source: elaborated by the authors.

Table 4 - Pumping cost from the maritime terminal to refinery  $r$  (US\$/m<sup>3</sup>).

$r$	REFINERY			
	A	B	C	D
$Cost_{p,r}^{CorPump}$	0.10	0.01	0.15	0.15

Source: elaborated by the authors.

Table 5 - Model constraints.

	REFINERY			
	A	B	C	D
LGP	10,000	30,000	42,000	70,200
N	5,600	25,000	36,000	60,000
K	33	30	26.7	30
D	27	20	25.5	23
AR	0.8	1.3	1.3	1.0
GO	6.0	22,5	10 <sup>-6</sup>	10 <sup>-6</sup>
VR	4.0	0	0	0
D	1,300	10 <sup>6</sup>	5,500	13,000
AR	10 <sup>6</sup>	10 <sup>6</sup>	17,000	10 <sup>6</sup>
GO	10 <sup>6</sup>	10 <sup>6</sup>	24,000	10 <sup>6</sup>
VR	4,300	10 <sup>6</sup>	21,000	10 <sup>6</sup>

Source: elaborated by the authors.

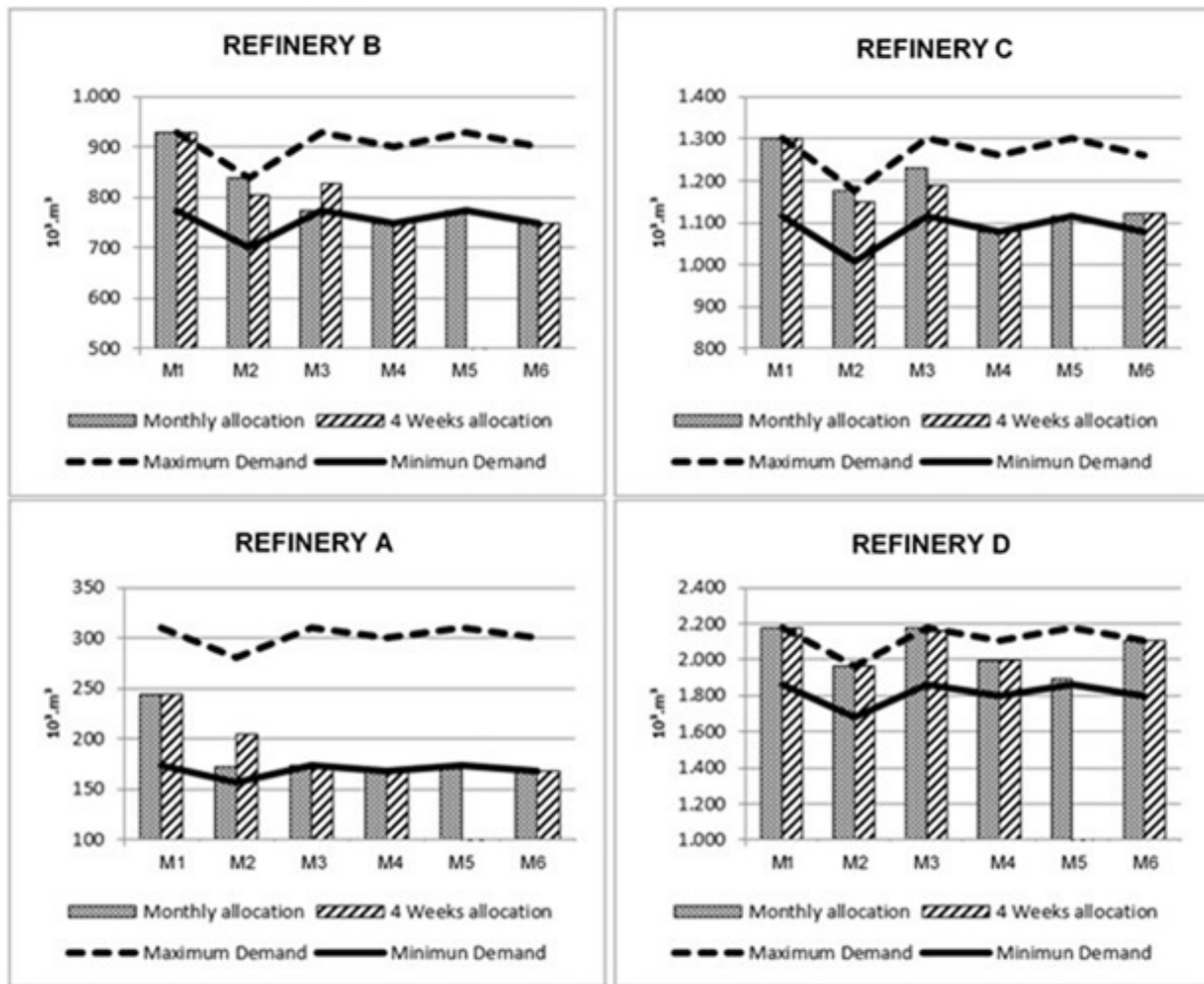
Figure 4 compares the resulting allocation for crude oils in each refinery in each month for the two cases under analysis: the whole month aggregated in a single time slot (planning) and its corresponding detailed version in which the entire month is weekly segmented into four time slots.

In this figure, dashed (full) lines indicate the upper (lower) bound for CDU volumetric processing charges in each refinery whereas checkered (hatched) bars denote the optimal solution found for this model variable with respect to the planning (plannuling) model. In principle, a feasible solution could not be determined for one instance of the plannuling model (month "M5"). This infeasibility was due to the impossibility of satisfying the minimum crude oil demand in REFINERY D in week 3 and in REFINERY B in weeks 1 and 2.

For this reason, M5 was not considered in the next evaluations. However, from this figure, the optimal analysis of the problem is noticed to result in high priority to maximize the processing charges in REFINERY D at the expense of lower processing rates in the remaining refineries, such as REFINERY A, even being the pumping cost between the maritime terminal and REFINERY D higher than that between the maritime terminal and REFINERY B or REFINERY A.

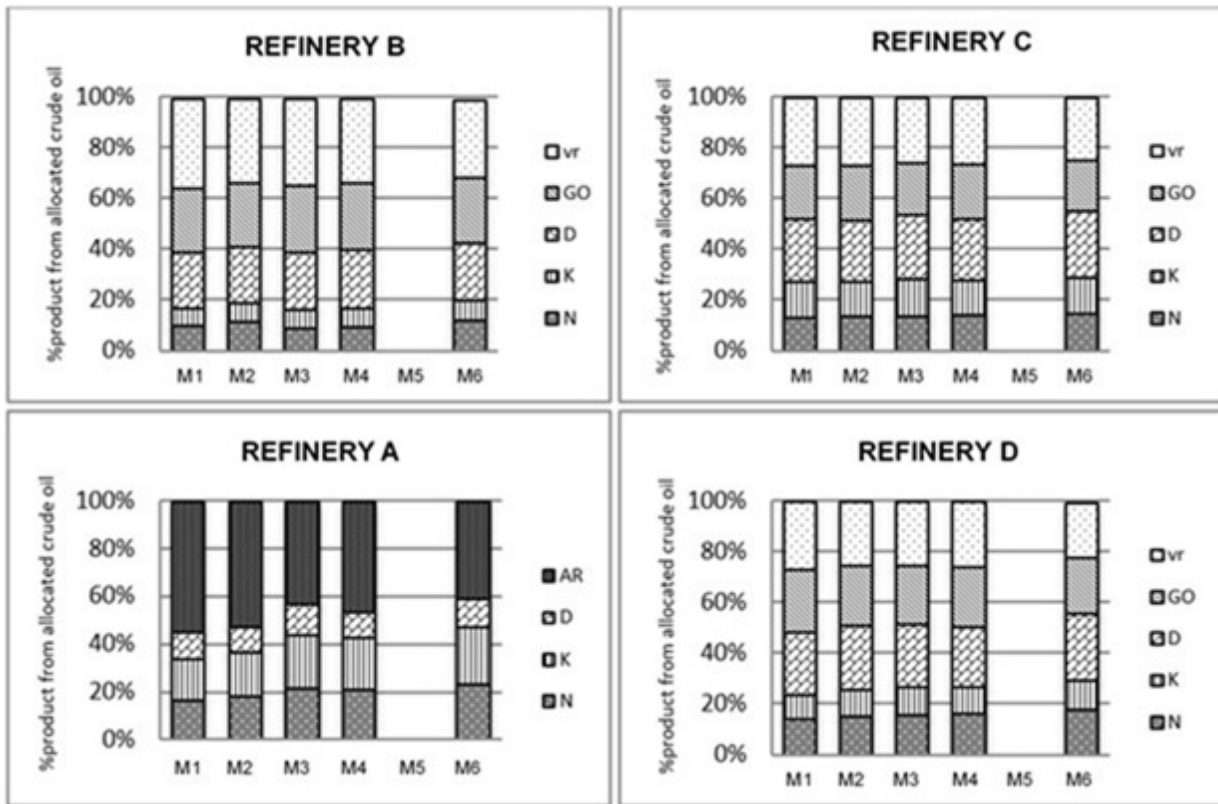
This is due to the significant economic trade-off between raw-material and products pricing, which surpasses the economic impact of crude oil transportation through oil pipelines. In fact, Figure 5 clearly shows that products with the lowest added-values (RAT or VR) have the highest participation in the REFINERY A production profile, while REFINERY D and REFINERY C (the refineries with the highest associated pumping costs) have a production profile characterized by larger amounts of products with higher added-value (naphtha, kerosene, diesel and gasoil). For this analysis, only the plannuling model was considered, once it gives the most realistic scenario between the two models studied. Therefore, the optimization model tried to saturate REFINERY D charge, even if the pumping costs are bigger there than in REFINERY A.

Figure 4 - Comparison of optimal refinery charging loads between the two modeling approaches



Source: elaborated by the authors.

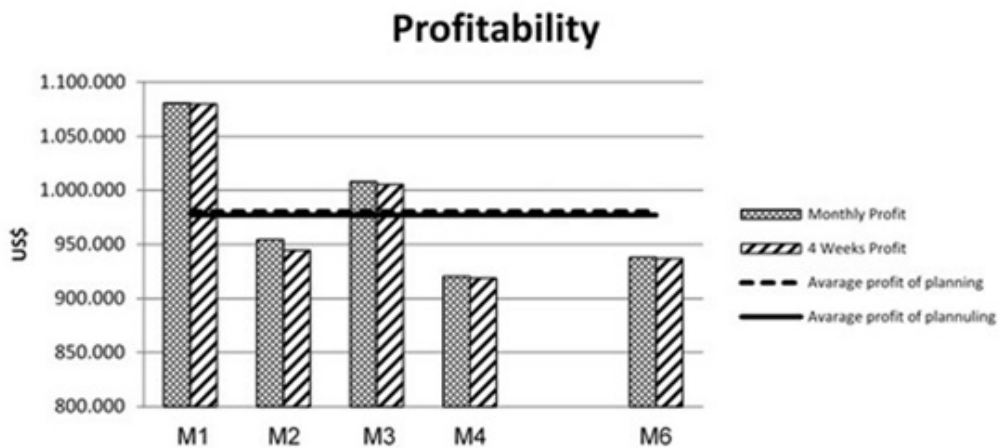
Figure 5 - Optimal production profiles according to the planning model (fictitious values).



Source: elaborated by the authors.

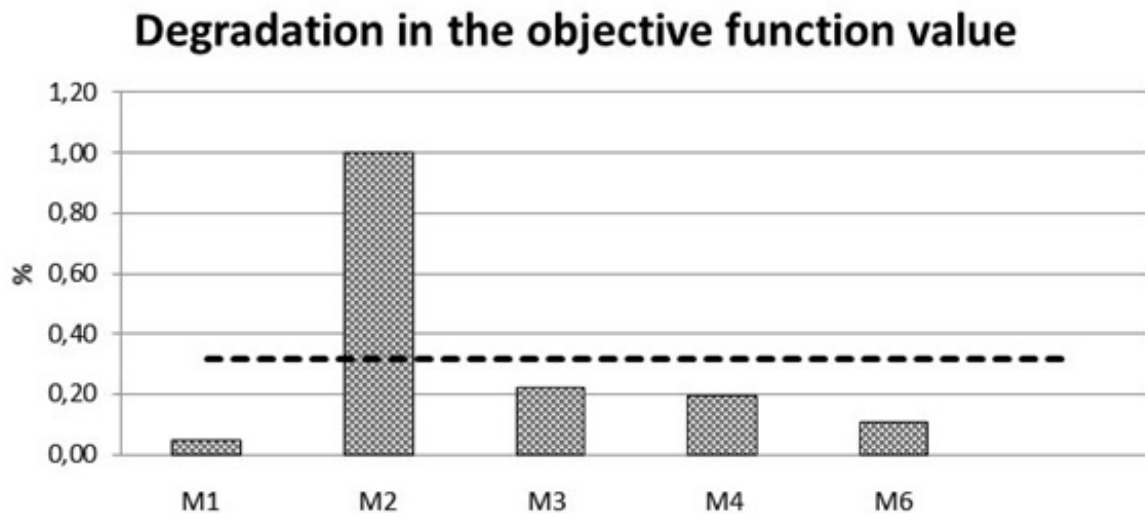
Figure 6 depicts the resulting monthly profitability associated with each modeling approach along the first semester of 2015 and their corresponding averages over this period. For each month, the corresponding gap in the objective function value (profit loss) between the planning and the planning models is depicted in Figure 7.

Figure 6 - System profitability related to both modeling approaches.



Source: elaborated by the authors.

Figure 7 - Degradation in the objective function value predicted by the one-month aggregated planning model when the system is solved regarding the weekly availability of crude oils. (-) denotes the average value.



Source: elaborated by the authors.

In terms of objective function value, the allocation suggested by the planning model was characterized by higher profits – around 0.32 % – as shown in Figure 7. As expected, the apparent degradation of the solution quality related to the planning model emerges as a primary consequence of the fact that this modeling approach is dimensionally larger (in terms of number of variables and constraints) and more constrained than the planning model. Specifically, the feasible space is reduced since we are introducing additional constraints on the crude oil availability along the month. Secondary factors that may contribute to such degradation are related to the fact that global optima are not warranted.

## 7 Conclusions

Here, we develop an NLP-based approach to efficiently solve an industrial-size optimization problem, the solution of which links strategic and operational decisions related to four highly integrated oil refineries. We demonstrate that the choice of the time aggregation level impacts the results of the optimization. However, depending on the problem instance considered, the planning model based on monthly time discretization can overestimate the profitability of the entire system by less than 1%, on average, in relation to its weekly discretized representation. Anyway, that efforts must be made to improve models and solution techniques to consider a lower level of time aggregation in the execution of tactical planning. This is because a finer discretization of the planning horizon helps to prevent optimization from producing an unfeasible production plan that cannot be executed at the production scheduling level.

Our work has several limitations, however. Firstly, the model proposed comprises important nonlinearities and, due to non-convexity issues, the solutions presented are potentially local optima. Secondly, since the model is a mere caricature of a complex system, the role of the human factor in interpreting the mathematical solution remains of paramount importance in this field. In particular, not all relevant oil qualities were considered in our modeling effort and some other important aspects were neglected. Here are included: the transportation times in long oil pipelines, the variations in pumping costs related to specific crude oil qualities (e.g., viscosity and density), the variations in the product yield profile in CDUs as a function of unity feed flowrate and alternative operation modes, and the physical constraints in the crude oil tank farm at each refinery and corresponding inventory costs.

Future work is planned to investigate more sophisticated solution strategies that explore the search for better local optimum points, such as the multiple-shooting strategy. With a set of more consistent results, a statistical basis can be created. Furthermore, the problem can be sophisticated and therefore be closer to the real problem, yielding an even more realistic solution.

## 8 References

BIEGLER, L.T.; GROSSMANN, I.E., **Retrospective on optimization**. Computers & Chemical Engineering Journal, v.28, n. 8, p.1169-1192, 2004.

CHARNES, A.; COOPER, W. W.; MELLON, B. **Blending aviation gasolines**. Econometrica, v. 22, p.135-159, 1952.

COSTA, F.L.P.; SOUSA, L.C.F.; JOLY, M.; TAKAHASHI, M.T.; MAGALHÃES, M.V.O.; MENDONÇA, P.N. **Sistema de otimização de misturas**. In: RIO OIL & GAS EXPO AND CONFERENCE, 2008. Rio de Janeiro; IBP, 2008.

CUTHRELL, J.E. ; BIEGLER, L.T., **On the optimization of differential-algebraic process systems**. AIChE Journal, v.3, n.38, p.1257-1270, 1987.

DANTIZG G. B., **Programming in a linear structure**. Econometrica, v.17, p.7374, 1949.

DRUD, A.S., **A System for large scale nonlinear optimization: reference manual for conopt subroutine library**. Bagsvaerd, Denmark: ARKI Cons. & Develop. A/S, 1996.

FEITAL, T.; LIMA, P.; PINTO, J.C.; SOUZA JR. M.B.; XAVIER G.; LIMA, M.J.; JOLY, M. **Rethinking petroleum products certification**. Journal of Petroleum Science and Engineering, 2013. V.2013. Article ID 594368. DOI:;<http://dx.doi.org/10.1155/2013/594368>.

GAREY, M.R. A; JOHNSON, D.S. Computers and intractability: a guide to the theory of NP-completeness. New York, EUA: W.H. Freeman and Company, 1979.

GROSSMANN, I. E. ; BIEGLER L.T. Future perspective on optimization. Computers & Chemical Engineering Journal, v.28, p.1193-1218, 2004. Part II.

HILLIER, F.S. AND LIEBERMAN, G.J. Introduction to operations research. 8th ed., New York, EUA : The McGraw-Hill Inc., 2005.

IACHAN, R. A Brazilian experience: 40 years using operations research at Petrobras, 2009.

IBM; IBM®; ILOG®; CPLEX®. Optimization Studio, Version 12 Release 2: Information Center, IBM, 2012. Available on: <http://pic.dhe.ibm.com/infocenter/cosinfoc/v12r2/index.jsp>. Access on: 04 abr.2014.

JOLY, M. Refinery production planning and scheduling: the refining core business. Brazilian Journal of Chemical Engineering, v. 29 n,2, p.371-384, 2012.

JOLY, M. ; PINTO, J.M. Mixed-integer programming techniques for the scheduling of fuel oil and asphalt production. Chemical Engineering Research and Design, v. 81, p. 427-447, 2003.

JOLY, M. ; PINTO, J.M., Role of mathematical modeling on the optimal control of HIV-1 pathogenesis. AIChE Journal, v.52, n.3, 856-884, 2006.

KARMAKAR, N. A new polynomial-time algorithm for linear programming, Combinatorica, v. 4, n.4, 373-395, 1984.

KELLY, J. D. Logistics: the missing link in blend scheduling optimization,2006.

KELLY, J.D. ; FORBES, J.F. Structured approach to storage allocation for improved process Controllability. AIChE Journal, v.44, n.8, p.1832-1840, 1998.

KONDILI, E.; PANTELIDES, C.C.; SARGENT, R.W.H. A general algorithm for scheduling batch operations. Computers & Chemical Engineering Journal, v.17, n2, p. 211-227, 1993.

LASSCHUIT W. ; THIJSSSEN N. Supporting supply chain planning and scheduling decisions in the oil and chemical industry. Computers & Chemical Engineering Journal, v. 28, p. 863-870, 2004.

LEE, H.; PINTO, J.M.; GROSSMANN, I.E.; PARK, S. Mixed-integer linear programming model for refinery short-term scheduling of crude oil unloading with inventory management. Industrial & Engineering Chemistry Research, v.35, p.1630-1996, 1996.

MAGALHÃES M.V.O. Refinery scheduling. Thesis (Doctorate in Philosophy) - Department of Chemical Engineering and Chemical Technology. University of London, London, UK, 2004.

MAGALHÃES M.V.O.; MORO L.F.L.; SMANIA P.; HASSIMOTO M.K.; PINTO J.M.; ABADIA GJ. SIPP – A solution for refinery scheduling. In: NPRA COMPUTER CONFERENCE, San Antonio, Texas , 1998.

MONIZ, S.; PÓVOA, A. P. B.; SOUZA J. P. New General Discrete-Time Scheduling Model for Multipurpose Batch Plants , [S.l.:s.n.], 2013.

MORO, L.F.L.; GROSSMANN, I.E., A mixed-integer model predictive control formulation for linear systems. *Comp. Chem. Eng.* v.55, n.8, p. 1-18, 2013.

NEIRO, M.S.N.; PINTO, J.M. A general modeling framework for the operational planning of petroleum supply chains. *Computers & Chemical Engineering Journal*, v.28, p. 871-896, 2004.

OTTINO, J.M. Complex systems. *AIChE Journal*, v.49, n.2, p. 292-299, 2003.

PANTELIDES, C.C. Unified frameworks for optimal process planning and scheduling. In: FOUNDATIONS of computer aided process operations- FOCAPO II, Colorado, EUA, 1994.

PINTO J.M.; JOLY M.; MORO L.F.L. Planning and scheduling models for refinery operations. *Computers & Chemical Engineering Journal*, v.24, p.2259-2276, 2000.

PINTO, J. M. ; NEIRO, S. M. S. A general modeling framework for the operational planning of petroleum supply chains. *Computers & Chemical Engineering Journal*, v.28, p.871-896, 2004.

ROCHA, R.; GROSSMANN, I. E.; ARAGÃO M. V. S. P. Petroleum allocation at PETROBRAS: mathematical model and a solution algorithm. *Computers and Chemical Engineering Journal*, v.2, p.123-213, 2009.

SHAH, N. K.; LI Z.; IERAPETRITOU M. G. Petroleum refining operations: key Issues, advances, and opportunities, 2010.

SYMONDS, G. H. *Linear programming: the solution of refinery problems*. New York: Esso Standard Oil Company, 1955.

VARMA V.A.; REKLAITIS G.V.; BLAU G.E.; PEKNY J.F. Enterprise-wide modeling & optimization – An overview of emerging research challenges and opportunities. *Computers and Chemical Engineering Journal*, v.31, p. 692-711, 2007.

VISWANATHAN J. ; GROSSMANN I.E., A combined penalty function and outer approximation method for MINLP optimization, *Computers and Chemical Engineering Journal*, v.14, n.7, p. 769-782, 1990.

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