



# REFINERY OPERATIONAL PLANNING: A CONVEX RELAXATION APPLICATION

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# **ABSTRACT**

The oil refining activity is certainly one of the most complex activities in the chemical industry. The complexity arises mainly from the nonlinear nature of the refining processes and the several possible configurations of these processes. In addition, these nonlinear terms are responsible for ruining convexity properties of the problem, thus, removing any guarantee concerning global optimality of the solutions. In this sense, one alternative to circumvent this drawback is to use convexification techniques, which render convex approximations of the original problem. The present work proposes the use McCormick envelopes to generate a convex approximation for the refinery operational planning problem. Numerical results obtained show that the proposed approach can ensure a good solution for the problem in study, even for cases where there was no solution available employing traditional methods.

**KEYWORDS.** Nonlinear programming. McCormick envelopes. Refinery operational planning.

P&G - OR in the Oil & Gas area.



The oil refining activity is one of the most complex activities in the chemical industry. The complexity arises mainly from the nonlinear nature of the refining processes and the several possible configurations of these processes. As a consequence of this complexity, planning of the oil refining operations must be aided by decision-making systems, especially those that employ mathematical programming – for example, RPMS (Bonner and Moore, 1979) and PIMS (Bechtel, 1993). In this way, mathematical programming plays a crucial role to assist the decision-making process in the oil supply chain.

In the literature, many operational planning models based on mathematical programming have been tested in real refineries. Gao *et al.* (2008) developed a mixed integer linear programming model (MILP) to address the production planning problem of a large-scale fuel oil-lubricant plant in China. The MILP proposed by Micheletto *et al.* (2007) optimizes the operation of a refinery plant in Brazil by considering mass and energy balances, operational mode of each unit, and demand satisfaction over multiple periods of time. Moro *et al.* (1998) developed a nonlinear planning model that maximizes the profit, which was applied to the particular case of diesel production in a Brazilian refinery. Other applications in Brazil can be found in Neiro and Pinto (2004, 2005). In their earlier work (Neiro and Pinto, 2004), the authors developed a general framework for modeling petroleum supply chains. The resulting multi-period mixed-integer nonlinear programming (MINLP) model was tested in a supply chain consisting of four refineries. A nonlinear integer programming application associated with uncertainty was investigated in the work by Neiro and Pinto (2005).

The mathematical models applied for optimization of refinery planning processes are typically nonlinear due to the consideration of material and property balances derived from product mixing activities. These nonlinear terms are responsible for ruining convexity properties of the problem, thus, removing any guarantee concerning global optimality of the solutions. In this sense, one alternative to circumvent this drawback is to use convexification techniques, which render convex approximations of the original problem.

The present work proposes the use McCormick envelopes (McCormick, 1976) to generate a convex approximation for the refinery operational planning problem. The McCormick envelopes technique can derive a convex approximation of the original nonconvex and nonlinear problem using a set of linear hyperplanes. Such a technique is especially suitable when the nonlinearities are caused by the presence of bilinear terms composed by the product of two variables with known bounds. The main benefits of using the McCormick envelopes are that the approximation obtained is linear (and, therefore, convex) and its precision is directly related with how tight the variable bounds are. In addition, it is possible to show that, when the optimal variable values are at their bounds, then the relaxation solution and the original problem solution are exactly the same. Karuppiah and Grossmann (2006) applied a similar technique in the water treatment problem. Gounaris and Misener (2009) discuss alternative convexification relaxation schemes for the pooling problem. A broad review regarding the use of these convexification techniques is provided in Floudas and Gounaris (2009).

The remainder of this paper is organized as follows. Section 2 presents the operational model for oil refinery. The convex envelopes of the nonlinear functions are presented in Section 3. Section 4 offers results for a case study using real data from the Brazilian oil industry and some conclusions are drawn in Section 5. Finally, Section 6 details the participation of the undergraduate student in this research.

#### 2. Oil Refinery Operational Planning Model

This section presents the mathematical formulation for the operational planning of oil refineries. This deterministic formulation is adapted from the model proposed by Ribas *et al.* (2012) by excluding all elements related to stochastic optimization. The proposed nonlinear programming model aims to maximize the profit of the oil refinery. The model allows for the proper selection of oil blending and considers an appropriate manipulation of intermediate



streams to obtain the final products in the desired quantities and qualities. The decision of oil blending combined with the operational modes for each process unit defines the yield and properties of all refined products. During one period of time more than one operational mode can be set for each process unit and the the combination of different modes allows the refinery to increase the yield of some refined product as desired. A series of nonlinear equations was modeled to obtain the correct property value of the intermediate products in order to precisely define the quality of the final products subjected to severe specifications. Definitions of sets, variables and parameters are provided in Tables 1 and 2, which are followed by the model formulation.

Table 1: Sets and variables

Sets		Sets	
Set of process units (u, u')	U	Storage tanks	$UA \subset U$
Set of operational modes $(c, c')$	С	Blending tanks	$UM\subset U$
Set of streams $(s, s')$	S	Process units (separation and conversion)	$UP \subset U$
Set of properties $(p, p')$ Time periods $\{n \mid n = 1,, T\}$	P T	Flows $(u,c,s,u',c')$ , where the par $(u,c)$ is origin and the par $(u',c')$ is the destine	$F \subset S$
Operational modes $c$ performed at unit $u$	$C_u \subset C$	Variables	
Properties $p$ of inlet flow at unit $u$	$PI_{u,c} \subset P$	Flow rate of stream $s$ between $(u,c)$ and $(u',c')$	$q_{u^{\prime},c^{\prime},s,u,c}^{t}$
Properties $p$ of outlet streams $s$ at unit $u$	$PO_{u,c,s} \subset P$	Inventory level at unit <i>u</i>	$vo_{u,c}^t$
Inlet streams $s$ at unit $u$	$SI_{u,c} \subset S$	Property $p$ of the inlet flow at unit $u$	$pi_{u,c,p}^t$
Outlet streams $s$ at unit $u$	$SO_{u.c} \subset S$	Property $p$ of the outlet stream $s$ at unit $u$	$po_{u,c,s,p}^t$
Tanks of raw materials	$UC \subset U$	Inlet flow rate at unit u	$qi^t_{u,c}$
Delivery units for final products	$UE \subset U$	Inlet flow rate of stream $s$ at unit $u$	$qis_{u,c,s}^t$
Tanks units (storage and blending)	$UT \subset U$	Outlet flow rate of stream $s$ at unit $u$	$qo_{u,c,s}^t$

Table 2: Parameters

Parameters	·	Parameters	
Product price	$PP_{u,s}^t$	Maximum offer of additional raw material	$QOA_{u,c,s}^t$
Cost of additional raw material	$CPA_{u,s}^t$	Oil offer defined by the tactical plan	$QOF_{u,c,s}^t$
Cost of fixed raw material	$\mathit{CPF}^t_{u,s}$	Minimum feed flow rate at unit u	$QL_u^t$
Inventory cost	$\mathit{CINV}_{u,s}^t$	Maximum feed flow rate at unit u	$QU_u^t$
Process unit yield	$YUP_{u,c,s,s}$	Property value $p$ of the outlet stream $s$ at process	$POUP_{u,c,s,s',p}^{t}$
Initial stock at unit u	$VOI_{u,c}^t$	unit $u$ as a function of inlet stream $s'$	
Minimum storing capacity at unit u	$VOL_{u,c}^t$	Property value p of initial stock	$POI_{u,c,p}^t$
Maximum storing capacity at unit u	$VOU_{u,c}^t$	Lower bound of outlet property $p$ at unit $u$	$POL_{u,c,s,p}^t$
Minimum demand	$DEML_{u,c,s}^t$	Lower bound of outlet property $p$ at unit $u$	$POU_{u,c,s,p}^t$
Maximum demand	$DEMU_{u,c,s}^t$		

#### **Model Formulation**

Objective Function (OF)

$$Maximize OF =$$

$$\sum_{u \in UE} \sum_{c \in C_u} \sum_{s \in SI_{u,c}} \sum_{t \in T} PP_{u,s}^t qis_{u,c,s}^t - \sum_{u \in UC} \sum_{c \in C_u} \sum_{s \in SO_{u,c}} \sum_{t \in T} CPA_{u,s}^t \left(qo_{u,c,s}^t - QOF_{u,c,s}^t\right) \tag{1}$$



$$-\sum_{u \in \mathit{UC}} \sum_{c \in \mathit{C}_u} \sum_{s \in \mathit{SO}_{u,c}} \sum_{t \in \mathit{T}} \mathit{CPF}_{u,s}^t \mathit{QOF}_{u,c,s}^t - \sum_{u \in \mathit{UA}} \sum_{c \in \mathit{C}_u} \sum_{s \in \mathit{SO}_{u,c}} \sum_{t \in \mathit{T}} \mathit{CINV}_{u,s}^t \mathit{vo}_{u,c}^t$$

## Process unit capacities

$$QL_{u}^{t} \leq \sum_{c \in C_{u}} qi_{u,c}^{t} \leq QU_{u}^{t}$$
 
$$\forall u \in \mathit{UP}, \forall t \in \mathit{T}$$

#### Material balances

$$qi_{u,c}^t = \sum_{(u',c',s,u,c)\in F} q_{u',c',s,u,c}^t \qquad \forall u \in \mathit{UP} \cup \mathit{UT}, \forall c \in \mathit{C}_u, \forall t \in \mathit{T}$$

$$qis_{u,c}^t = \sum_{(u',c',s,u,c) \in F} q_{u',c',s,u,c}^t \qquad \forall u \in \mathit{UP} \cup \mathit{UT} \cup \mathit{UE}, \forall c \in \mathit{C}_u, \forall s \in \mathit{SI}_{u,c}, \forall t \in \mathit{T} \qquad (4)$$

$$qo_{u,c,s}^t = \sum_{(u,c,s,u',c') \in F} q_{u,c,s,u',c'}^t \qquad \forall u \in \mathit{UP} \cup \mathit{UT} \cup \mathit{UC}, \forall c \in \mathit{C}_u, \forall s \in \mathit{SO}_{u,c}, \forall t \in \mathit{T} \qquad (5)$$

$$vo_{u,c}^{t} = VOI_{u,c}^{t} + vo_{u,c}^{t-1} + qi_{u,c}^{t} - \sum_{s \in SO_{u,c}} qo_{u,c,s}^{t}$$
 
$$\forall u \in UA, \forall c \in C_{u}, \forall t \in T$$
 (6)

$$\sum_{s \in SC_{u,s}} qo_{u,c,s}^t = qi_{u,c}^t \qquad \forall u \in UM, \forall c \in C_u, \forall t \in T$$
 (7)

# Balance in the process unit

$$qo_{u,c,s}^t = \sum_{s' \in SI_{u,c}} qis_{u,c,s'}^t YUP_{u,c,s,s'} \qquad \forall u \in UP, \forall c \in C_u, \forall s \in SO_{u,c}, \forall t \in T$$
(8)

## Supply plant constraints

$$QOF_{u,c,s}^t \le qo_{u,c,s}^t \le QOF_{u,c,s}^t + QOA_{u,c,s}^t \qquad \forall u \in UC, \forall c \in C_u, \forall s \in SO_{u,c}, \forall t \in T$$
 (9)

#### Stock constraints

$$VOL_{u,c}^t \le vo_{u,c}^t \le VOU_{u,c}^t$$
  $\forall u \in UA, \forall c \in C_u, \forall s \in SO_{u,c}, \forall t \in T$  (10)

## Demand constraints

$$DEML_{u,c,s}^t \le qis_{u,c,s}^t \le DEMU_{u,c,s}^t \qquad \forall u \in UE, \forall c \in C_u, \forall s \in SI_{u,c}, \forall t \in T$$
 (11)

#### Property value for the output stream at the process unit

$$po_{u,c,s,p}^{t}qo_{u,c,s}^{t} = \sum_{s \in SI_{u,c}} qis_{u,c,s}^{t} YUP_{u,c,s,s} POASSAY_{u,c,s,s',p}^{t}$$

$$\tag{12}$$

$$\forall u \in \mathit{UP}, \forall c \in \mathit{C}_u, \forall s \in \mathit{SO}_{u,c}, \forall p \in \mathit{PO}_{u,c,s}, \forall t \in \mathit{T}$$

## Property value for the output stream at the tank unit

$$po_{u,c,s,p}^{t}\left(VOI_{u,c}^{t} + vo_{u,c}^{t-1} + qi_{u,c}^{t}\right) = POI_{u,c,p}^{t}VOI_{u,c}^{t} + po_{u,c,s,p}^{t-1}vo_{u,c}^{t-1} + pi_{u,c,p}^{t}qi_{u,c}^{t}$$

$$\forall u \in UA, \forall c \in C_{u}, \forall s \in SO_{u,c}, \forall p \in PO_{u,c,s}, \forall t \in T$$

$$(13)$$

# Property value for the inlet flow at all types of unit

$$pi_{u,c,p}^{t}q_{u,c}^{t} = \sum_{(u',c',s,u,c)\in F} q_{u',c',s,u,c}^{t}po_{u',c',s,p}^{t} \qquad \forall u\in \mathit{UP}\cup\mathit{UT}, \forall c\in \mathit{C}_{u}, \forall p\in \mathit{PI}_{u,c}, \forall t\in \mathit{T} \qquad (14)$$

## Property specification

$$POL_{u,c,s,p}^{t} \le po_{u,c,s,p}^{t} \le POU_{u,c,s,p}^{t} \qquad \forall u \in UT, \forall c \in C_{u}, \forall s \in SO_{u,c}, \forall p \in PO_{u,c,s}, \forall t \in T$$
 (15)



$$q_{u',c',s,u,c}^t, qis_{u,c,s}^t, qi_{u,c}^t, qo_{u,c,s}^t, vo_{u,c}^t \in \Re^+, pi_{u,c,p}^t, po_{u,c,s,p}^t \in \Re$$
(16)

The refinery oil supply is defined by the tactical plan of the company, and is represented in the model as the parameter  $QOF^t_{u,c,s}$ . The model also considers the purchase of additional oil at the spot market defined as the parameter  $QOA^t_{u,c,s}$ . The oil purchase in the spot market is a model decision used to adjust the oil blending according to the quantity and quality of the products on demand. The other main decisions are related to the refinery operations, such as flows between units  $(q^t_{u',c',s,u,c})$ , inventory level  $(vo^t_{u,c})$ , and refined products properties  $(pi^t_{u,c,p}$  and  $po^t_{u,c,s,p})$ . The objective function (Equation 1) maximizes the operating profit. The profit includes

The objective function (Equation 1) maximizes the operating profit. The profit includes the revenue from the products sales less the cost of purchasing oil in the spot market, the cost of raw materials from the tactical plan and the inventory costs.

Equation (2) controls the feed flow rate of the unit u. Equation (3) describes the mass balance at the inlet stream s of the unit u ( $qi_{u,c}^t$ ). Equation (4) represents the mass balance at the inlet stream s of the unit u ( $qi_{u,c,s}^t$ ). Equation (5) describes the mass balance at the outlet stream s of the unit u ( $qo_{u,c,s}^t$ ). The stock balance in the storage unit is represented by Equation (6). Equation (7) corresponds to the mass balance for the blending units. Equation (8) represents the process unit, where the outlet flow rate of stream s ( $qo_{u,c,s}^t$ ) is a function of the feed flow rate of stream s' and the process unit yield.

Equation (9) limits the outlet flow rate for raw material tanks. Fixed (tactical plan decision) and additional (spot market) raw materials are available. The refinery consumes all the fixed raw material and purchases the additional raw material necessary for its operation. Equation (10) represents the inventory level for product tanks at every time period t. Equation (11) limits the inlet flow rate for the final products in the delivery units.

The nonlinear constraint used to calculated the property value of all intermediate stream and final products are defined in Equations (12), (13) and (14), where the multiplication of the variables flow  $(qo^t_{u,c,s})$  and property value  $(po^t_{u,c,s,p})$  are needed. Equation (12) defines the property value for the outlet stream at the separation and conversion units. Equation (13) refers to the property value for the outlet stream at the tank unit, which consider the stock at the time interval t-1 and the inlet flow rate at the time interval t. Equation (14) defines the properties of the inlet flow for all types of units. Equation (15) specifies the property range for the final products.

#### 3. McCormick Envelopes for Nonlinear Functions

Equations (12), (13) and (14) are nonlinear and also the cause of the solution space non-convexity. Bearing this in mind, we will focus on relaxing these constraints in order to replace the original feasible space by its convex hull. These relaxations will be performed using underestimating convex and overestimating concave envelopes for the bilinear terms. These envelopes are known as McCormick envelopes (McCormick, 1976). The bilinear term will be replaced by a new variable, and it will be limited by four inequalities that compose the envelopes. The relaxed model will be linear, and therefore convex, which yields a problem that is much easier to solve. Unfortunately, its solutions might not be feasible in the original problem. Nevertheless, this solution can be used as an starting point for the original model. Moreover, the solution value of the relaxation serves as an upper bound for the global maximum.

For the sake of clarity, we present an example to illustrate how to apply the McCormick envelopes. Suppose that there is a constraint of the form (17), where f(x) and g(y) are linear functions.

$$f(x) + g(y) + xy = 0 (17)$$

The product xy will be replaced by a new variable w. This new variable w will be limited by four new constrains, (18), (19), (20) and (21), where the first two compose a convex envelope and the last two, a concave one. Finally, equation (17) will be removed and equation (22) will be



added to the model together with the envelopes defined by 18, 19, 20, and 21. It is important to highlight the necessity of known bound for the variables to define the envelopes. Furthermore, if the bounds are tighter, the bilinear terms will be approximate more precisely the envelopes.

$$w \ge xY^{lo} + X^{lo}y - X^{lo}Y^{lo} \tag{18}$$

$$w \ge xY^{up} + X^{up}y - X^{up}Y^{up} \tag{19}$$

$$w \le xY^{up} + X^{lo}y - X^{lo}Y^{up} \tag{20}$$

$$w \le xY^{lo} + X^{up}y - X^{up}Y^{lo} \tag{21}$$

$$f(x) + g(y) + w = 0 (22)$$

Equations (23), (24), and (25) are the relaxed versions of the nonlinear equations (12), (13) and (14) respectively. Constrains (26) to (29) are the envelopes for the product of  $po_{u,c,s,p}^tqo_{u,c,s}^t$ . The other envelopes are defined in a similar way.

Property value for the output stream at the process unit

$$poqo_{u,c,s,p}^{t} = \sum_{s' \in SI_{u,c}} qis_{u,c,s}^{t} YUP_{u,c,s,s'} POASSAY_{u,c,s,s',p}^{t} \ \forall u \in UP, \forall c \in C_{u}, \forall s \in SO_{u,c}, \forall p \in PO_{u,c,s}, \forall t \in T$$

Property value for the output stream at the tank unit

$$povo_{u,c,s,p}^{t,t-1} + poqi_{u,c,s,p}^{t} + po_{u,c,s,p}^{t}VOLI_{u,c}^{t} = POI_{u,c,p}^{t}VOLI_{u,c}^{t} + povo_{u,c,s,p}^{t-1,t-1} + piqi_{u,c,p}^{t}$$

$$\forall u \in UA, \forall c \in C_{u}, \forall s \in SO_{u,c}, \forall p \in PO_{u,c,s}, \forall t \in T$$

$$(24)$$

Property value for the inlet flow at all types of unit

$$piqi_{u,c,p}^t = \sum_{(u',c',s,u,c)\in F} poq_{u',c',s,u,c,p}^t \qquad \forall u \in UP \cup UT, \forall c \in C_u, \forall p \in PI_{u,c}, \forall t \in T$$
 (25)

Envelopes for pogo

$$poqo_{u,c,s,p}^{t} \ge po_{u,c,s,p}^{t}QO_{u,c,s}^{t,lo} + PO_{u,c,s,p}^{t,lo}qo_{u,c,s}^{t} - PO_{u,c,s,p}^{t,lo}QO_{u,c,s}^{t,lo}$$

$$\forall u \in UP, \forall c \in C_{u}, \forall s \in SO_{u,c}, \forall p \in PO_{u,c,s}, \forall t \in T$$

$$(26)$$

$$poqo_{u,c,s,p}^{t} \geq po_{u,c,s,p}^{t}QO_{u,c,s}^{t,up} + PO_{u,c,s,p}^{t,up}qo_{u,c,s}^{t} - PO_{u,c,s,p}^{t,up}QO_{u,c,s}^{t,up}$$

$$\forall u \in UP, \forall c \in C_{u}, \forall s \in SO_{u,c}, \forall p \in PO_{u,c,s}, \forall t \in T$$

$$(27)$$

$$poqo_{u,c,s,p}^{t} \leq po_{u,c,s,p}^{t}QO_{u,c,s}^{t,up} + PO_{u,c,s,p}^{t,lo}qo_{u,c,s}^{t} - PO_{u,c,s,p}^{t,lo}QO_{u,c,s}^{t,up}$$

$$\forall u \in UP, \forall c \in C_{u}, \forall s \in SO_{u,c}, \forall p \in PO_{u,c,s}, \forall t \in T$$

$$(28)$$

$$poqo_{u,c,s,p}^{t} \leq po_{u,c,s,p}^{t}QO_{u,c,s}^{t,up} + PO_{u,c,s,p}^{t,up}qo_{u,c,s}^{t} - PO_{u,c,s,p}^{t,up}QO_{u,c,s}^{t,up}$$

$$\forall u \in UP, \forall c \in C_{u}, \forall s \in SO_{u,c}, \forall p \in PO_{u,c,s}, \forall t \in T$$

$$(29)$$

## 4. Results

An industrial scale study using real data from the Brazilian industry was used to evaluate the performance of the proposed model and methodology. The methodology discussed previously in Section 3 was compared to directly solving the model. The solvers used by the proposed methodology are CPLEX 12.1 for the relaxed model and CONOPT 3 for the nonlinear model, when solving directly, the solver used was CONOPT 3. The models were implemented in GAMS 3.9.1 software package and a computer using an Intel i7 3770 processor with 8.0 GB RAM was used for all computational results described in this section. Seven cases were analyzed that differs in price and limits of oils offers, price and limit of products demands, units'



capacities, streaming yields, among others parameters.

The results for the proposed methodology are resumed in Table 3, where the "Relaxed Model" shows the results using the McCormick envelopes and the "Original Model" shows the results of the NLP model considering the relaxed solution as an initial point. The results for solving directly are presented in Table 4. Table 5 gives the comparisons of the proposed methodology with solving directly ("Heuristic comparison") and also shows the gap between the methodology solution and the global solution upper bound ("Global comparison").

**Table 3.** Proposed methodology results

		Relaxed Model			Original Model			
	#Variables	#Constraints	Solving Time (s)	OFV (million \$)	#Variables	#Constraints	Solving Time (s)	OFV (million \$)
Case 1	2543	1403	0.78	19.969	823	973	0.047	19.969
Case 2	1463	1144	0.75	14.987	667	815	0.063	13.833
Case 3	1930	1447	0.672	14.209	868	1045	0.635	13.821
Case 4	2525	1978	0.812	16.422	1103	1348	0.093	15.958
Case 5	3274	1777	0.765	20.418	994	1213	0.047	17.544
Case 6	2445	1315	0.749	11.413	725	889	0.061	10.665
Case 7	1889	2163	0.764	5.073	667	815	0.046	5.008

**Table 4.** Directly solving model

	#Variables	#Constraints	Solving Time (s)	OFV (million \$)
Case 1	823	973	0.826	infeasilbe
Case 2	667	815	0.862	infeasilbe
Case 3	868	1045	0.777	infeasilbe
Case 4	1103	1348	0.857	infeasilbe
Case 5	994	1213	0.765	infeasilbe
Case 6	725	889	0.812	infeasilbe
Case 7	667	815	0.842	0.853

**Table 5.** Comparisons

	Heuristic (	Comparion	Global	
	time (%)	OFV (%)	Comparision (%)	
Case 1	0.12	Not available	0	
Case 2	-5.68	Not available	-7.7	
Case 3	68.21	Not available	-2.73	
Case 4	5.6	Not available	-2.83	
Case 5	6.14	Not available	-14.08	
Case 6	-0.25	Not available	-6.56	
Case 7	-3.8	486.96	-1.29	

# 5. Conclusions

The purpose of this paper was to discuss the problem of oil refining. A model was proposed to incorporate different types of refinery units, market variables and properties specifications. Since this model was nonconvex and nonlinear, and therefore difficulty to solve without a good initial point, a methodology using McCormick's envelopes was created. The methodology allowed solving the model in all tested cases while improving the objective function with no real loss in time in the case that were already possible to solve without it.

Furthermore, another achievement of the methodology is the possibility of comparing the solution to an upper bound of the global solution, and it's shown that the solution is at most 14.08% less than the global in the worst tested case, the mean gap is 5.03%, and in one case, the local solution found is also a global maximum since it is equal to the upper bound.

## 6. Undergraduate Student Activities

The present work was sent to compete in the Prêmio de Iniciação Científica (PIC) and is part of a research project aiming to develop a refinery operational planning system. The main stages of the project were:

- 1. Training and qualification of staff.
- 2. Development of mathematical model for the refinery operational planning.
- 3. Development of application for reading input data and writing the results in XML format.
- 4. Propose methodologies and solutions to solve infeasibility problems and to improve the solution quality, to obtain the global optimum of the problem.

The undergraduate student who is competing for the PIC attended the four stages of the project. In the first stage of training the student has studied the literature regarding the operational planning of oil refineries and participated in the course Introduction for refining processes and



practical courses in GAMS modeling and database in Microsoft Access. In the second stage of the mathematical model development the student participated in the equations and results validation. In the third stage also validated the application developed to read the input data and writing the results in XML format.

The fourth step is the proposed solution to the model of nonlinear programming (NLP) resulting from the second step. In this activity the students had their main contribution to the research project developing a methodology for solving the problem using the NLP technique of McCormick envelopes (1976). The methodology initially proposed by the advisors and fully implemented by the student. During the implementation phase the student also envisioned improvements of the initial idea of the methodology, which ensured even greater benefits with respect to the performance of the proposed method. This methodology aims to define, from the NLP model, convex approximations for the feasible region through the McCormick envelopes. These envelopes was used to obtain a linear relaxation (and hence convex) of the original problem. This convex relaxation was then used to obtain a good initial solution for nonlinear optimization method employed. Note that the success of the proposed methodology is closely linked to quality of the initial solution provided, a solution that is not trivially available in large complexity problems, as the one discussed in this work. Numerical results obtained by the student show that their approach can ensure a good solution for the problem in study, even for cases where there was no solution available employing traditional methods.

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#### References

**Bechtel,** *PIMS (Process Industry Modeling System) User's manual. Version 6.0.* Houston, TX: Bechtel Corp., Houston, 1993.

**Bonner and Moore,** RPMS (Refinery and Petrochemical Modeling System): a system description, Bonner and Moore Management Science, Houston, NY, 1979.

**Floudas, C. A., and C. E. Gounaris.** A review of recent advances in global optimization. Journal of Global Optimization 45.1 (2009): 3-38.

Gao, Z., Tang, L., Jim, H. & Xu, N. (2008) An optimization model for the production planning of overall refinery. *Chinese Journal of Chemical Engineering*, 16(1), 67-70.

Gounaris, Chrysanthos E., Ruth Misener, and Christodoulos A. Floudas. Computational comparison of piecewise—linear relaxations for pooling problems. *Industrial & Engineering Chemistry Research* 48.12 (2009): 5742-5766.

**Karuppiah, Ramkumar, and Ignacio E. Grossmann.** Global optimization for the synthesis of integrated water systems in chemical processes. *Computers & Chemical Engineering* 30.4 (2006): 650-673.

**McCormick, Garth P.** Computability of global solutions to factorable nonconvex programs: Part I—Convex underestimating problems. *Mathematical programming* 10.1 (1976): 147-175.

**Micheletto, S., Carvalho, M. and Pinto, J.** (2007) Operational optimization of the utility system of an oil refinery. *Computers and Chemical Engineering*, 32(1-2), 170-185.

**Moro, L., Zanin, A. and Pinto, J.** (1998) A planning model for refinery diesel production. *Computers and Chemical Engineering*, 22, 1039-1042.

**Neiro, S. and Pinto, J.** (2004) A general modeling framework for the operational planning of petroleum supply chains. *Computers and Chem. Engineering*, 28(6-7), 871-896.

**Neiro, S. and Pinto, J.** (2005) Multiperiod optimization for production planning of petroleum refineries. *Chemical Engineering Communications*, 192(1), 62-88.

**Ribas, G., Leiras A. and Hamacher, S.** (2012) Operational planning of oil refineries under uncertainty. *IMA Journal of Management Mathematics*, doi:10.1093/imaman/dps005.