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Optimization of H_2 Production in a Hydrogen Generation Unit

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Abstract: This article presents the results of the use of advanced process control algorithm to optimize the H_2 production of Henrique Lage Refinery (REVAP) located in the state of São Paulo, Brazil. The control methodology is applied to the second Hydrogen Generation Unit (HGU) of the Refinery and consists of optimizing its production in order to guarantee the hydrogen supply for the refinery's header without production loss. The designed controller had the support of dynamic simulation for disturbances modelling and identification which contributed for the improvement of the control strategy. The results in this paper represents the application of the control methodology in the real plant.

Keywords: Advanced Process Control; Optimization, Hydrogen Generation.

1. INTRODUCTION

The benefits of Advanced Process Control (APC) projects are well known by engineers of both industry and academy. These benefits include not only costs savings but also considerable reduction of key process indicators variability leading to an overall improvement of the process stability. The APC key to success lies in the possibility of handling several constraints while dealing with disturbances rejection. Also, modern control and optimization algorithms are successful where process dynamics are complex and highly integrated, leading to degradation of the classical PID controllers performance, Delaney [2012].

Engineers must have in mind that APC should not be seen as an alternative or substitute for classical control, but more as a system integrator, working alongside PID loops to improve process efficiency. The APC projects are successful where the classic control strategies are not efficient. These projects usually require experienced personnel, since the modern engineering exercises behind their development are not accessible to everyone. Even so, the economic and operational benefits achieved with APC are beyond the implementation costs. Some of these benefits are discussed in Nello [2011]. An economically based analysis of how APC projects improve systems' performance may be found in Zanin et al. [2007] and some issues concerning the importance of trained personnel are found in King [2012]. An interesting explanation of the APC development history and also a contemporary view of APC use can be read in Delaney [2012]. Insights on the main difficulties found in some applications as well as reasons why part of APC projects fail to deliver proper results are given by Lodolo et al. [2012].

This paper presents an application that shows the advantages of APC implementation in a hydrogen generation unit (HGU) of an important Brazilian refinery facility. The APC was designed to reject several disturbances and maintain the hydrogen header pressure in safe operational conditions. The result is the complete zeroing of production loss through vent valves designed to protect against high pressure. The process is detailed in section 2. Section 3 discusses the optimization issues considered for the unit and section 4 presents some results regarding economic achievements and operational improvements of the implemented APC in the real plant. A conclusion is given to summarize the questions raised throughout the paper and give insights for further improvements.

2. PROCESS DESCRIPTION

2.1 H_2 Header Configuration

The REVAP's hydrogen supply header consists of three integrated H_2 generation units feeding five hydrotreating (HDT) units. The hydrogen is used in HDT process to remove sulphur, nitrogen and other contaminants in the Diesel and Naphtha streams. The H_2 flow required by the HDT unit is a function of the processed feed and part of the H_2 used in the process is recovered in the high/low pressure separator vessels, returning to the process as recycle hydrogen. The H_2 make-up compressors are designed to complement the hydrogen flow required by the hydrotreating process.

The first HGU unit (HGU-I) was designed to attend the Diesel, Naphtha and Kerosine units, which were the first HDT units in the refinery. In the last couple of years the refinery's modernization projects were responsible for the startup of the three new HDTs: The Gasoil HDT

(HDT-GOK), the Naphtha Coker HDT (HDT-NK) and the Cracked Naphtha Hydrodessulphurization (HDS-NC) units . Also, the Continuous Catalytic Reforming unit (CCR) was designed to treat the HDT-NK outlet stream and obtain Reformed Naphtha. Hydrogen is a sub-product of the catalytic reforming process. In order to attend the hydrogen demanded by the new HDT units, a second HGU (HGU-II) was designed to complement the production of the first HGU. In early 2012, the three hydrogen generators were integrated in one header with the purpose of improving reliability and minimizing the effects of non-programmed shutdown of these units. Vent valves in the hydrogen generation units outlet streams are set for high pressure control. Figure 1 shows the refinery's hydrogen header current configuration.

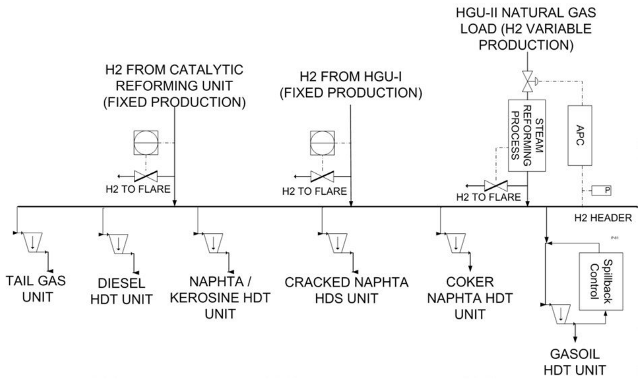

Fig. 1. H_2 Header of Henrique Lage refinery

The produced hydrogen is sent to each HDT unit through the make-up compressors. The HDT-GOK is the greater hydrogen consumer and processes the FCC's Light Cycle Oil (LCO) and Coker Gasoil (GOK). There's a special control system in the HDT-GOK H_2 make-up compressor composed of a spillback surge vessel that absorbs the header pressure minor variations whenever a mass flow unbalance takes place. This system is actioned when rapid intervention on the HDT hydrogen consumption is necessary to avoid higher header pressure drop.

2.2 Hydrogen Generation Unit

Figure 2 illustrates the hydrogen generation process. The H_2 header pressure controller sets the desired natural gas and steam flow rates that compose the reformer's feed. Both natural gas and steam flow setpoints are calculated by the steam to carbon ratio *crosslimit* control loop, with the purpose of keeping the reforming process under safe operational conditions. A lower ratio may result in coker formation in the reformer's radiation section, whereas higher ratios decrease the reformer's thermal efficiency, [CENPES, 2004].

The steam to carbon ratio is illustrated in Figure 3. The H_2 header pressure controller output signal sets the desired carbon molar flow. This molar flow sets the saturated steam flow according to the defined ratio. The crosslimit control loop is designed to guarantee an excess of steam over the defined ratio during transitory feed changes. It means that the natural gas flow increases *after* and decreases *before* the steam flow whenever setpoint changes for the natural gas are required.

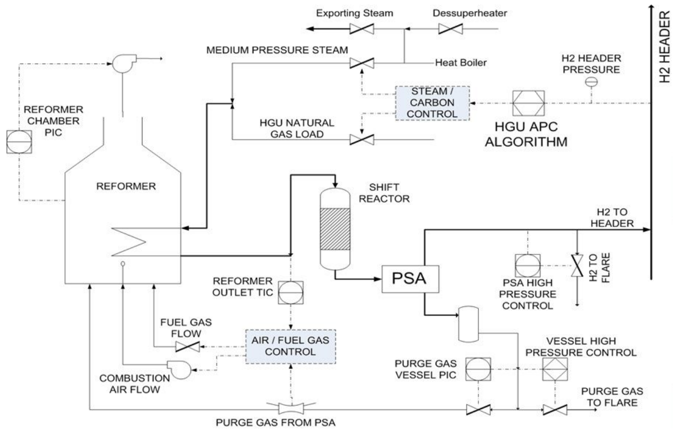

Fig. 2. Hydrogen Generation Unit

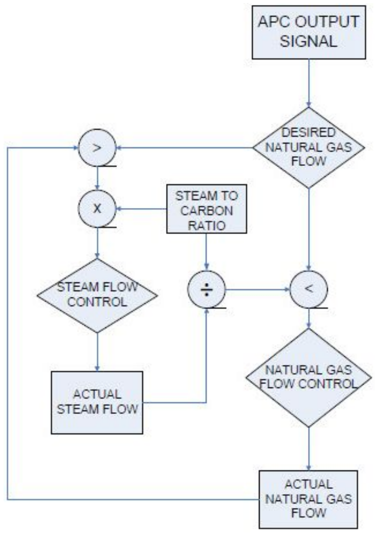

Fig. 3. Steam to Carbon Ratio Control Flowchart

In the reformer's radiation section, the saturated steam and the natural gas react under high temperature conditions. The steam reforming reactions are shown in equation (1), [CENPES, 2004]:

$$
\begin{aligned}
& C_nH_m + H_2O \rightarrow nCO + [(2n+m)/2]H_2 \\
& CO + H_2O \leftrightarrow CO_2 + H_2 \\
& 2CO \leftrightarrow C + CO_2 \\
& CO + H_2 \leftrightarrow C + H_2O \\
& CH_4 \leftrightarrow C + 2H_2
\end{aligned}
\tag{1}
$$

The energy demanded by the steam reforming reaction is supplied by the fuel gas burning under O_2 excess environment. The burning process is controlled by an air / fuel gas crosslimit loop that guarantees an air flow excess over the fuel gas flow in order to prevent the formation of hazardous environment. The air/fuel gas control loop is illustrated in Figure 4.

The reformer's outlet temperature controller sets the energy required by the reforming process. This energy is

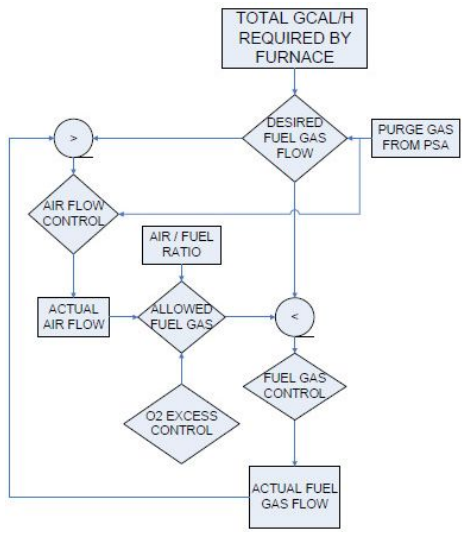

Fig. 4. Air / Fuel Gas Control Flowchart

converted in setpoint for the fuel gas flow controller. As an O_2 excess is necessary to avoid incomplete burning, the crosslimit loop increases the air flow before the fuel gas flow whenever an energy demand increases and reduces the fuel gas flow before the air flow in the opposite scenario. The minimization of the O_2 excess is an important optimization parameter on industrial furnaces as low excess may result in hazardous environment, whilst high excess reduces the furnace's thermal efficiency, [Campos and Teixeira, 2006].

The reformed gas flows to the shift reactor in order to convert part of the CO presented in the gas into CO_2 with the purpose of improving H_2 separation in the *Pressure Swing Adsorption* (PSA) system. The exothermic reaction inside the shift reactor is expressed by equation (2), [CENPES, 2004]:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad \Delta H^o_{298} = -41.02kJ/mol \quad (2)$$

The PSA separates the reformed gas into two streams: One stream containing high purity hydrogen and the other stream is the purge gas that is sent back to the reformer for burning. The produced H_2 is sent to the refinery's header to supply the HDT's demand. A purge gas surge vessel homogenizes the purge gas stream from the PSA before sending it to the purge gas burners in the reformer. A vent valve is also set in the vessel outlet to protect against high pressure, sending excess flow to the flare system.

3. OPTIMIZATION

The optimization project for the HGU consists basically in balancing the H_2 demand, avoiding excess H_2 venting. Also, the purge gas resulted from the PSA must be entirely processed in the reformer avoiding energy loss to flare. In other words, optimizing H_2 generation means minimize production loss to flare. It represents not only energy savings but also compliance with modern environmental regulations [Xu et al., 2009]. For REVAP's optimization project two important tools were used: The disturbance rejection efficiency of APC techniques and the process modelling capability of dynamic simulators.

3.1 Advanced Process Control

The designed APC is a two-layer optimizer with the stationary layer running a Quadratic Programming (QP) algorithm used for steady-state optimization and constraints handling. This layer generates the setpoints and targets of the manipulated and controlled variables of the dynamic layer, which uses a *Dynamic Matrix Control* (DMC) algorithm, [Cutler and Ramaker, 1980] for targets tracking and disturbance rejection. The two-layer optimization strategy is illustrated in Figure 5. The QP algorithm, [Garcia and Morshedi, 1986] solves the cost function given by equation (3), [Zanin et al., 2007]:

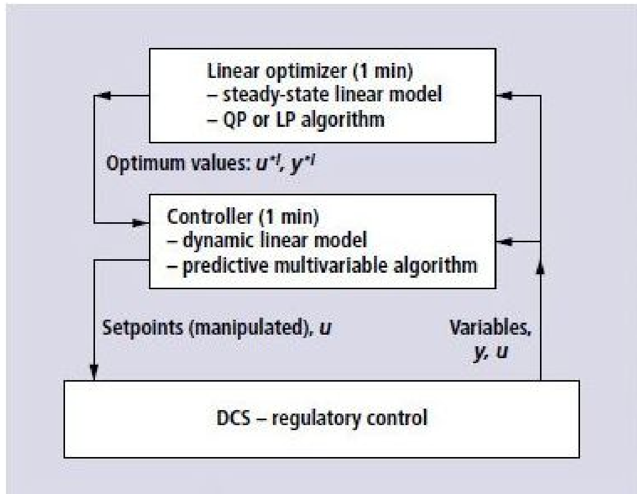

Fig. 5. APC with Two-layer strategy [Rotava and Zanin, 2005]

$$\min_{\Delta U, SCV} -W_1 \Delta U + \|W_2 \Delta U\|_2^2 + \|W_3 SCV\|_2^2 \quad (3)$$

subject to:

$$\Delta U = U_S - u_{at}$$
$$U_S^{inf} \leq U_S \leq U_S^{sup}$$
$$Y_S^{inf} \leq Y_S + SCV \leq Y_S^{sup}$$

where $W_1 = diag[\frac{\partial f_{eco}}{\partial u_1}, \frac{\partial f_{eco}}{\partial u_2}, \ldots, \frac{\partial f_{eco}}{\partial u_n}]$ is the diagonal matrix of the economic coefficients of the manipulated variables (MVs), W_2 is the diagonal matrix of the suppression factors of the MVs and W_3 is the diagonal matrix of weights for the *slack* variables (SCV) used for softening the constraints. These three matrices are, in fact, the tuning parameters of the optimization layer. U_S is the vector containing stationary values of the MVs and Y_S is the vector of stationary values of the controlled variables (CVs). The dynamic layer receives the targets calculated by optimizer and runs the multivariable predictive control (MPC) algorithm for optimal targets tracking and disturbances rejection, keeping the process inside its operational range. The MPC algorithm control law is shown in equation (4), [Rotava and Zanin, 2005]:

$$\min_{\Delta U_i, i=1,\ldots,nl} \sum_{j=1}^{nr} \|W_4(Y_p - Y_l)\|_2^2 + \sum_{i=1}^{nl} \|W_5 \Delta U_i\|_2^2 + \sum_{i=1}^{nl} \|W_6 \left(u_{i-1} + \sum_{k=1}^{i} \Delta U_k - u^* \right) \|_2^2 \quad (4)$$

subject to:

$$-\Delta U^{max} \leq \Delta U \leq \Delta U^{max};\ j = 1, \ldots, nl$$

$$u^{inf} \leq u_{i-1} + \sum_{i=1}^{j} \Delta U_i \leq u^{sup};\ j = 1, \ldots, nl$$

where W_4 is the diagonal matrix of weights for the CVs, W_5 is the diagonal matrix of the suppression factors for the MVs and W_6 is the diagonal matrix of weights for the predicted controller outputs. These three matrices are the tuning parameters of the dynamic layer. Y_p is the vector of predictions of the CVs, u^* and Y_l are the targets calculated by the optimization layer.

The HGU's controlled variable is the H_2 header pressure, which is a function of the hydrogen flow demand. The HDT-GOK hydrogen make-up compressor's spillback PIC control signal is used to anticipate the header pressure drop. The manipulated variable is the HGU natural gas feed. The constraints are given by the operational range of the variables in the crosslimit control loops. Table 1 lists the MVs and CVs of the APC project, where ↑ means direct action and ↓ means reverse action:

Table 1. Manipulated and controlled variables

	MVs
	H_2 Header PIC control signal
CVs	
H_2 header PIC process variable	↑
HDT-GOK spillback PIC control signal	↑
Steam FIC setpoint and control signal	↑
Furnace air FIC setpoint and control signal	↑
Furnace air PIC setpoint	↑
Furnace fuel gas PIC setpoint	↑
Furnace chamber PIC control signal	↑
Export steam TIC control signal	↑
PSA inlet temperature	↑

Changes in the flow rate of the HDT's feeds are responsible for the variation on the H_2 flow demand and they are sent to the controller as disturbance variables. Also, the HDT-GOK works in high severity conditions, i.e., high pressure and temperature due to the characteristics of the feed, the nature of the catalysts and strong reactions that occurs inside the reactors. This unit runs in two modes: The $S500$ run produces Diesel with maximum sulphur concentration of $500ppm$ (parts per million); the $S10$ run produces Diesel with maximum sulphur concentration of $10ppm$. The $S10$ run experiments a considerable elevation on the H_2 consumption due to an increase in the process severity, which is expressed mainly by the reactors **WABT** (*Weighted Average Bed Temperature*). In order to improve the APC performance, this variable is also considered for feedforward control. The disturbances of the APC project are listed in Table 2:

Table 2. APC disturbance variables

	CV
	H_2 Header PIC process variable
DVs	
LCO and Coker Gasoil flow rate	↓
Coker light Naphtha flow rate	↓
Light Cracked Naphtha flow rate	↓
Heavy Cracked Naphtha flow rate	↓
HDT-GOK *WABT*	↓
CCR H_2 production	↑
HGU-I H_2 production	↑

The DMC algorithm control law is intrinsically capable of predicting and anticipating the effects of the disturbances in the H_2 header pressure, improving the overall stability of the process by reducing its variability. However, due to safety and operational issues, the hydrogen flow of the other generators cannot be manipulated. The high importance of these models for reliability and continuous operation of the APC led to the use of dynamic simulation for modelling and identification of H_2 production loss.

3.2 Dynamic Simulation

A simulator project, using RSI's Indiss® software, was designed to guide engineers throughout the H_2 header integration process and provide safety analysis. The project contains the evolved units and incorporates the spillback surge vessel control system, illustrated in Figure 6.

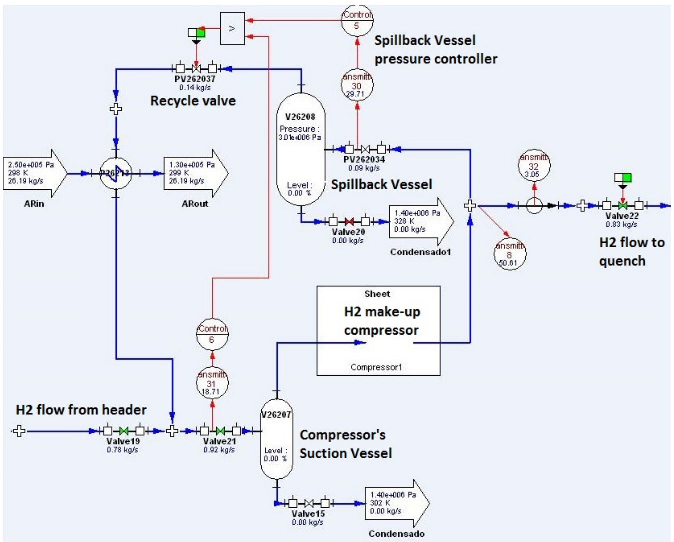

Fig. 6. H_2 make-up compressor's spillback control system

The system consists of an override scheme between the pressure controller at the hydrogen make-up compressor's discharge and a low pressure controller at the compressor's suction, manipulating the recycle valve whenever the HDT-GOK H_2 consumption is higher than the header production. The spillback vessel equalizes the HDT's reactors pressure, providing H_2 during short unbalance periods. The importance of the dynamic simulation lies in the possibility of obtaining system's behavior insights over several different scenarios [Al-Dossary et al., 2008]. Also, it provides the disturbance models for the particular variables that would not have identification tests performed in the real plant due to reliability issues [Luyben, 2012].

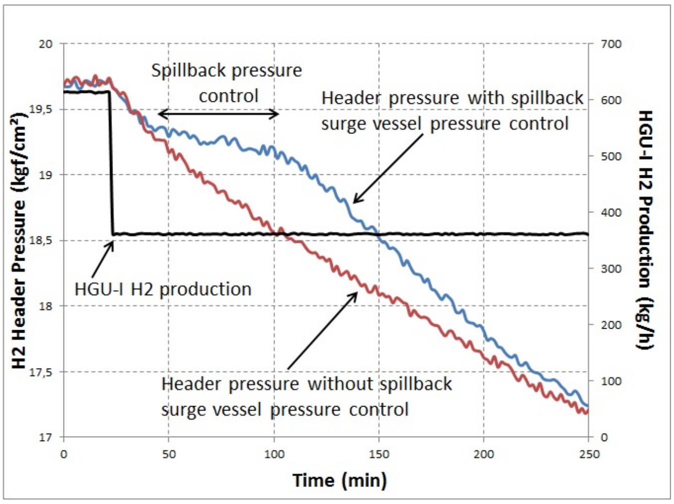

Fig. 7. H_2 header pressure simulation with and without spillback control

It is important to give simulator the most reliable data and documentation on disposal. The documentation necessary for a proper simulation scheme is described in [Psarrou et al., 2007]. Figure 7 shows a simulated scenario considering a decreasing H_2 flow production from the first HGU. It shows the effects on the header pressure as well as the moment when the spillback control acts avoiding higher pressure drop and stabilizing the system. A second scenario, where the spillback control is not present was simulated for comparison. The spillback surge vessel is able to stabilize the header pressure for short periods, resulting in a first order model behavior within the APC's prediction horizon.

4. RESULTS

An example of the APC feedforward action is shown in Figure 8. It shows the anticipation on the header pressure drop (controlled variable, right axis) due to an increase of the processed LCO in the Gasoil HDT (disturbance, left axis). The HGU natural gas flow rate (manipulated variable, left axis) is increased to compensate the future changes in the HDT's H_2 consumption (left axis). The

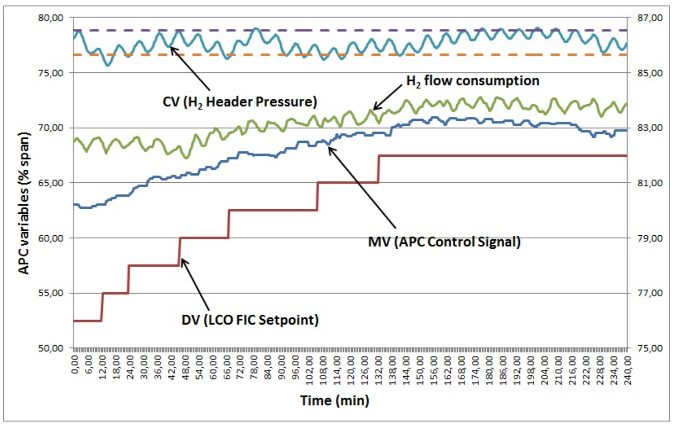

Fig. 8. APC Feedforward control action - Feed changing

dashed lines are the CV's control limits. All variables are expressed in percentage of span. The APC sampling time is T_S = 1min with a prediction horizon of nr = 120min and control horizon of nl = 8min.

Figure 9 shows another example of feedforward action of the APC. The control signal (right axis) is increased to compensate the HGU-I H_2 flow production to header decay (right axis). Also, it is possible to see the effect of the spillback control in the header pressure (left axis), avoiding higher pressure drop while the H_2 production is increased. The pressure dynamics is very close to the simulated result shown in Figure 7.

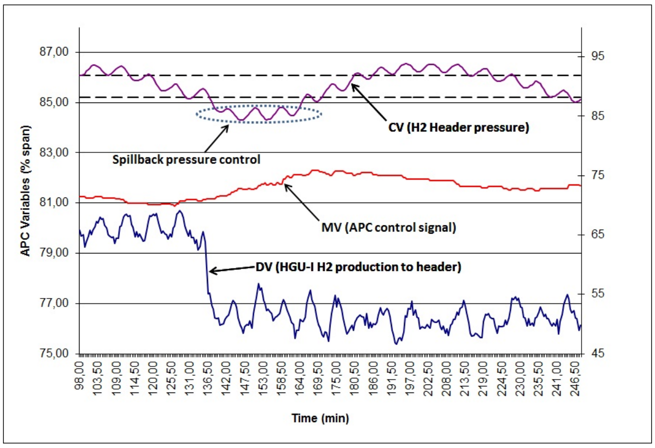

Fig. 9. APC Feedforward control - H_2 production decay

The APC project economic analysis is illustrated in the Figures 10 and 11 for a 4-month period after commissioning when compared to the manual operation during the previous six months. The solid line in Figure 10 shows the daily average H_2 loss to flare, in kg/h. The dashed line represents the average loss before and after the APC startup and the bar lines are the mean vent opening, in %. It is noticeable the APC capability of preventing energy loss through the manipulation of the HGU feed in order to match the H_2 flow demand.

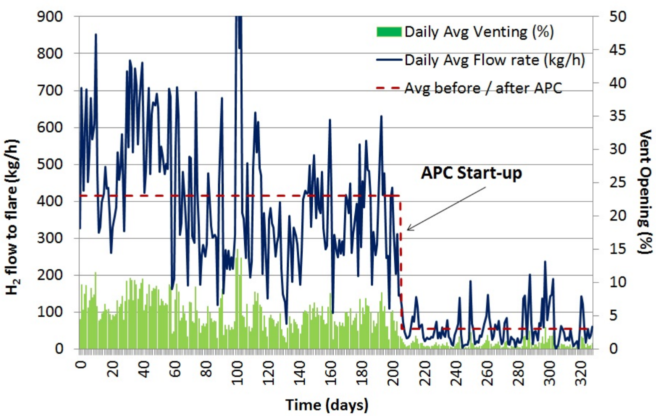

Fig. 10. H_2 loss to flare

Optimization is better represented by the Figure 11. The bar lines are the daily average natural gas flow that was processed in excess, resulting in the H_2 venting. This calculation considers the ratio between the natural gas and the produced H_2 flows. The reduction of the excess flow is the main economic variable used to evaluate the project yields.

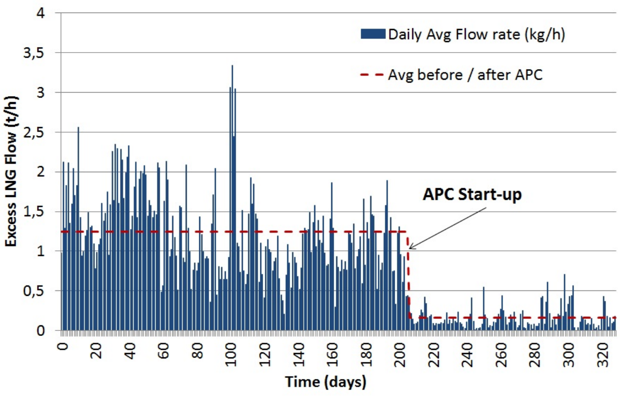

Fig. 11. Excess processed natural Gas

The calculated data results support the graphics evaluation of the APC's performance. Table 3 shows the average of the main variables taken into account for the project's economic-based analysis before and after the APC commissioning. The H_2 venting experimented a 86.11% reduction, which represents a decrease of 86.30% in the excess natural gas that was processed.

Table 3. Unit's performance before / after APC

	Before APC	After APC	Δ
H_2 venting	$415.99 kg/h$	$57.74 kg/h$	86.11%
Excess Natural Gas	$1.48 ton/h$	$0.20 ton/h$	86.30%

The project economic yield is given by Equation (5):

$$E = C_{NG} * \left(1 + \frac{\bar{Q}_{FG}}{\bar{Q}_{NG}}\right) * \sigma * \bar{Q}_{H_2} \quad (5)$$

where C_{GN} is the natural gas cost, in USD/ton, σ is the H_2 / natural gas stoichiometric ratio, equation 1, $\bar{Q}_{FG}$ is the nominal fuel gas flow to reformer, $\bar{Q}_{NG}$ is the nominal HGU natural gas feed and $\bar{Q}_{H_2}$ is the average H_2 flow rate, in ton/day. Based on the results presented in Table 3 for a methane-rich natural gas ($\sigma = 3.0$) and considering the average for the prices in the evaluated period the estimated economic savings for the APC project is $USD\ 23,300/day$, approximately $USD\ 8,400,000/year$. The numbers reinforce the importance of the advanced control for the refinery's energy balance management.

5. CONCLUSION

The paper results illustrate the economic benefits of the design and implementation of advanced control strategies applied to a hydrogen generation unit. These benefits come from the optimization of the processed feed to match the H_2 production according to the HDTs demand. A dynamic simulator was used for modelling the H_2 pressure header response to production variation, giving reliable models for the APC project. Future improvements include new manipulated variables in order to maximize CO to CO_2 conversion, improving the H_2 separation into the PSA system and maximizing the natural gas to hydrogen ratio.

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