

Validation of a hydrogen network RTO application for decision support of refinery operators

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Abstract: The validation process of a real-time optimiser (RTO) of a refinery hydrogen network is studied in this paper. The analysis focuses on the RTO utility for operators' decision support, due to process and equipment uncertainties, such as actual hydrogen demand and hydrocarbons (HC) loads. The validation underpins on the analysis of shortlisted key network variables, comparing actual reconciled (REC) and RTO figures. This methodology is applied to: a high hydrogen demand scenario (period 1), and a low hydrogen demand scenario (period 2). The RTO showed better solutions than REC for both periods. However, the gap between RTO and REC was larger at lower hydrogen demands, due to better usage of hydrogen purification membranes by the RTO than operators. Additionally, other important information for operators was provided by the RTO, such as optimal HC loads, least gas purges and optimal hydrogen production. Hence, the application of the RTO for aiding operators' decisions was successfully validated. Nonetheless, some challenging limitations appeared and are discussed. This is the case of: a more sensible account of low purity header lower bound, and incorporation of Lagrange multipliers to the analysis. These improvements may lead future work on the subject.

Keywords: real-time optimisation, decision support tool, hydrogen network, network optimisation

1. INTRODUCTION

Process network optimisation tools have been promoted in the last years, however their application is still difficult due to complex interactions of individual process units within the network. Moreover, the fact that automatic, semi-automatic and manual equipment coexist in the network makes the process network real-time optimisation even more complicated. At the same time, process optimisation improvements are highly encouraged by industries, driven by environmental and economic concerns. This is particularly the case of crude oil refineries, being their hydrogen (H_2) network one of the most studied cases in literature (De Prada et al., 2017; Elsherif, Manam and Kansah, 2015; Jhaveri, Mohanty and Khanam, 2014; Kumar, Gautami and Khanam, 2010; Méndez et al., 2008; Towler et al., 1996).

A refinery H_2 network is required to provide H_2 for sulphur removal of hydrocarbons (HC) to produce diesel and gasoline fuels. Sulphur removal occurs in different types of hydrodesulphurisation process units throughout the network. And the H_2 is fed to the network through hydrogen process units (HPU). Therefore, maximum benefit is obtained by processing maximum HC loads at minimum HPU costs (i.e.: minimum H_2 production). However, due to the fact that in reality processes are not static, real-time optimisation (RTO) becomes a key asset, in particular for operators.

This work analyses the validation process of an RTO developed by the Process Control and Supervision research group of the University of Valladolid (CSP, n.d.) in cooperation with Petronor SA (Petronor, n.d.). The application was successfully implemented at Petronor refinery, in Muskiz, Basque Country, Spain.

1.1 Hydrogen network case study

The refinery hydrogen network comprises four producers and fourteen consumers, a simplified schematic of the network is presented in Fig. 1 (Gomez, 2016). Based on previous data reconciliation techniques applied by Sarabia et al. (2012) raw data from the process network are validated, obtaining actual robust plant figures and REIs (Galan et al, 2017). A first principle model of the network along with plant data is used to obtain estimators that consider uncertainty of measurements where redundancy is available, while providing estimations of unmeasured variables (e.g.: molecular weights of streams, H_2 content, etc). The reduced model comprises: mass balances, equilibriums in gas-liquid separators, gas recycle loops and other first principle equations of the network units (more information on the model is provided by De Prada et al, 2017 & Gomez, 2016). The reconciliation model comprises circa 4400 variables and circa 4700 equality and inequality constraints. Once data has been reconciled, the optimal distribution

problem runs underpinned on reconciled estimations and incorporating some process units' loads and two H_2 producers as manipulated variables (MV). As a result, the optimisation comprises circa 2000 variables and circa 1800 equality inequality constraints. Both problems are NLP and are implemented on GAMS using IPOPT solver running on a dedicated PC (3.47 GHz 32 bits i5 CPU) at Petronor, and the overall execution takes circa 15 minutes. In summary, the RTO applies real-time reconciliation and optimisation to determine optimal network conditions to the H_2 distribution problem using the process economy as objective function.

Additionally, the network is controlled by a commercial dynamic matrix controller (DMC), which runs on six process units. The optimisation module of the DMC actually implements the RTO management policies rather than the set points. Figure 2 shows a simplified control scheme of the H_2 network, and the different levels integrated. It should be noticed that control room operators may adjust manually DMC variables' limits according to actual process unit conditions and planning objectives.

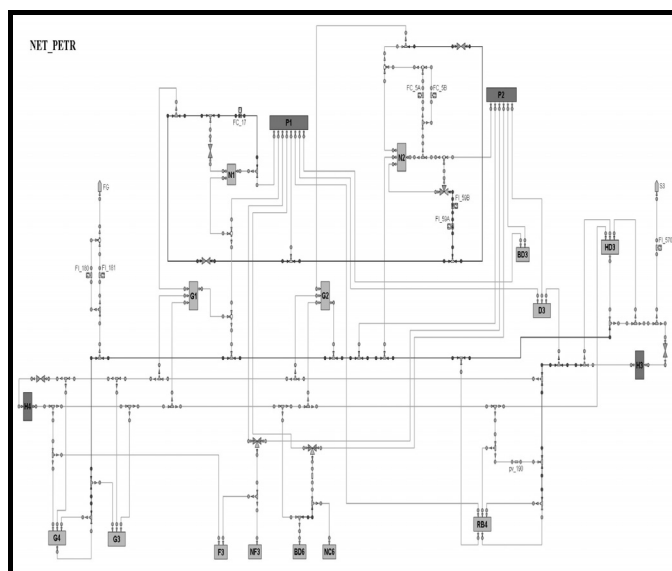


Fig. 1. Schematic of Petronor hydrogen network. Source: Gomez (2016).

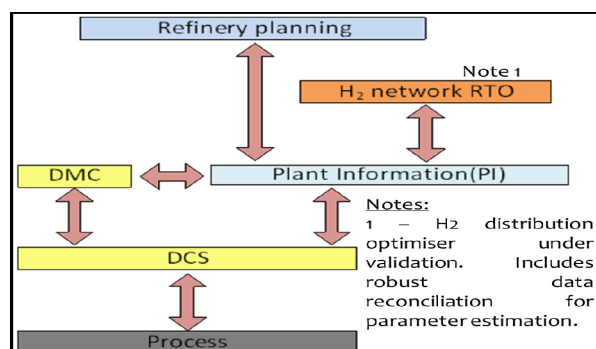


Fig. 2. Simplified control levels integration scheme.

More details of the application deployed and its architecture are presented by De Prada et al. (2017).

1.2 Aims

This research work is aimed at presenting, and analysing a refinery hydrogen RTO validation process, with respect to its utility as a decision support tool at network level for operators.

Particularly, it is aimed at analysing the most relevant variables of the hydrogen network, highlighting those that impact most in the process economy.

2. METHODOLOGY

2.1 RTO variables studied

The reconciled (REC) and optimised (OPT) results from the RTO are used for the analysis. The RTO cost function for the optimisation is based on the process economy (1). In particular, is formulated as a maximisation form accounting HC loads as benefits and H_2 production as costs. The process operational and safety constraints at plant and network level are satisfied as well ($h(x)$, $g(x)$ in 1).

$$\begin{aligned} &\max f(x) \\ &\text{subject to :} \\ &h(x)=0 \quad f \equiv \text{process economy} = \text{benefits} - \text{costs} \quad (1) \\ &g(x) \leq 0 \quad h, g \equiv \text{process model and constraints} \end{aligned}$$

Where,

benefits: HC loads · HC price, €/h (HC processed benefits)

costs: H_2 produced · H_2 cost, €/h (H_2 production costs)

A screening process of high network impact variables was conducted previous to this work, obtaining a set of preliminary variables for studying. This allowed focusing on a reduced group of variables, rather than attempting to analyse all at once. Variables that represented MV and controlled variables (CV) of the DMC were shortlisted. In addition, variables of material and H_2 balances at network level were shortlisted as well. In Table 1 a summary of the variables shortlisted for further analysis are shown. It should be born in mind that most RTO variables have REC and OPT values, and each gas stream its own H_2 purity as well as flow rate. The only exceptions were ten HC loads that were only used at the parameter estimation for these were imposed feeds from upstream units. Hence, there were not degrees of freedom in the optimisation problem.

The analysis was conducted on the understanding that those variables in the framework of the DMC (CV and MV) were already controlled following a set point from a cost function. However, this cost function did not necessarily represent the actual process economy, which RTO did partially reflect (1).

Purification membranes (Z1 and Z2), not considered in the DMC model, cannot be operated autonomously from the

control room and require the intervention of field operators. However, they affect the global H_2 mass balance by increasing H_2 purity in the network, and therefore were analysed. Although membranes were modelled in accordance with (2), the analysis is presented in terms of the permeate stream (H_{2perm}) for space constraint reasons.

Table 1. Summary of shortlisted variables analysed.

*Variables present in the model. HPU: Hydrogen process unit; PG: purge gas; FGH: fuel gas header.

	Quantity	DMC*	RTO*
HPU	2	Yes	Yes
HC loads	14	4	4
PG to FGH	1	Yes	Yes
Membranes	2	No	Yes

$$H_{2perm} = a * \frac{PG}{FD} + b * H_2FD + c$$

$$H_{2perm} \equiv \text{Hydrogen permeate purity, } (\% H_2) \quad (2)$$

$$PG \equiv \text{Membrane purge flowrate, } (Nm^3 h^{-1})$$

$$FD \equiv \text{Membrane feed flowrate, } (Nm^3 h^{-1})$$

$$H_2FD \equiv \text{Hydrogen feed purity, } (\% H_2)$$

$$a, b, c \equiv \text{membrane characteristic parameters}$$

2.2 Validation process

Firstly, RTO results were checked against DMC variables seeking inconsistencies from both and correcting them, where applicable. From this iterative work, several improvements resulted to both RTO and DMC. Therefore, at some point that RTO results were validated from an applicability point of view, i.e.: RTO propositions could actually be implemented in the process units, the optimal distribution proposed by the RTO was analysed focusing on its relevance to operators' decisions.

Secondly, a set of resource efficiency indicators (REIs) was previously developed and studied by Galan et al (2017) for this network. In particular, this work uses HC REIs to assess the optimisation figures with respect to HC loads in the H_2 network (Fig. 3).

Finally, two periods of significantly different H_2 network demand were chosen for performing the final stage of the validation process of the RTO. Therefore, figures of the variables were analysed and discussed under high and low H_2 network demands.

Results of this last stage of the validation process are presented and discussed in the next section.

3. RESULTS AND DISCUSSION

All figures presented in this work are in percentages instead of absolute SI units due to confidentiality reasons.

3.1 Network balances

Is important to notice that, both operation periods show high process units utilisation rates reflected on HC REIs (shown in Fig. 3). For instance, HC REIs were mostly above 0.99 (period 1) and over 0.985 (period 2). Therefore, HC loads in the network were in general close to the optimum, though they achieved maximums of 0.996 (period 1) and 0.995 (period 2). Additionally, Fig. 1 shows that period 1 was steadier than period 2. Possibly due to several attempts of increasing HC loads in period 2, which is reflected in HC REI's variations (e.g.: between executions 30-46).

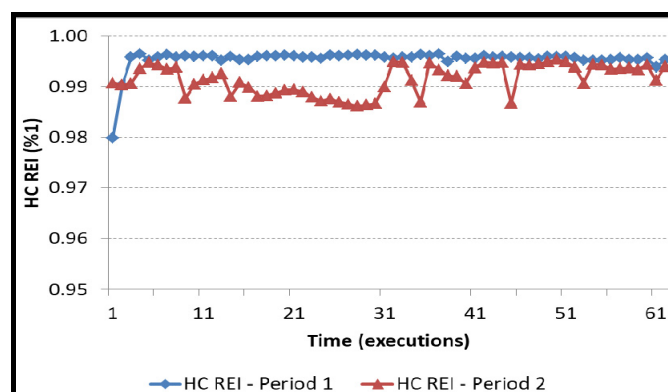


Fig. 3. HC REIs of periods 1 and 2.

Additionally, differences between H_2 demands are seen in Fig. 4, where reconciled and optimal H_2 productions figures of both periods are presented together. In Fig. 5 the differences between REC and OPT ($\Delta[REC-OPT]$) is presented. Is important to point out that period 1 presents larger H_2 production $\Delta[REC-OPT]$ from execution 13 to 26, and from 28 to 46. From execution 47 onwards both periods present similar performance in terms of their $\Delta[REC-OPT]$. At the same time, their H_2 productions figures approach until they end up together close to 95% at execution 58. From there period 2 continues rising up to 99.2 % [REC] (99.8 % [OPT]), while period 1 drops down to 91.2 % [REC] (88.9 % [OPT]). Relating Fig. 2-3 is seen that higher REC-OPT gaps appear at higher H_2 production rates.

The previous suggests that the RTO proposed H_2 productions differ more with the DMC (actual H_2 network management) at higher production rates (period 1) than at lower production rates (period 2). An explanation for this gap is that RTO incorporated to its model the effect of Z1 and Z2, while the DMC is unable to consider their effect. The membranes seem to make a difference at high H_2 production rates, where H_2 might be scarce and increasing H_2 purity in the LPH saves HP H_2 for other producers. At low rates the cost of operation of the membranes does not payoff H_2 production savings, since HC loads are already at their maximum. Therefore, membranes, and more generally LPH purification units, perform a critical role in the network operation when the refinery is processing HCs with a high H_2 demand, typically the sourer and more aromatic the worse. Under the previous scenarios (e.g.: period 1), membranes purification provides either H_2 production savings or space to increase HC load.

While the former has a moderate impact in the process economy, the latter has a huge impact (5 orders greater).

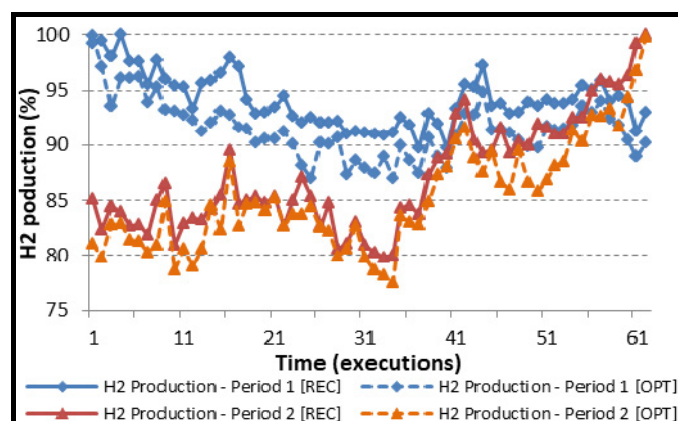


Fig. 4. Reconciled (REC) and optimal (OPT) H₂ production registered for periods 1 and 2 (P1-2).

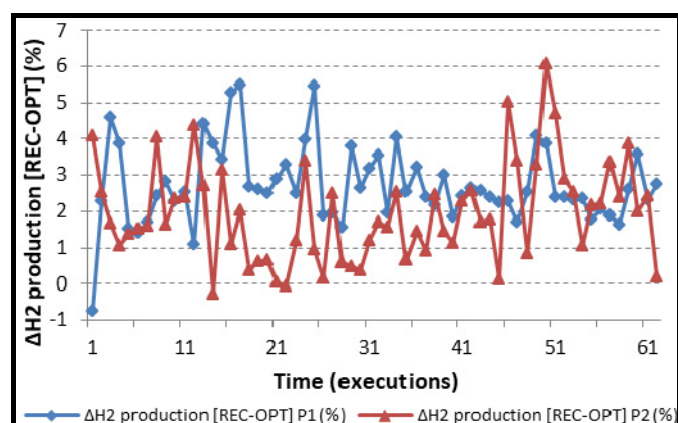


Fig. 5. H₂ Production difference between OPT and REC figures for periods 1 and 2 (P1-2).

3.2 Low purity header gas (LPHG)

A key control element in the H₂ network is the LPH gas purge (LPHG) to the fuel gas header (FGH). In principle, LPHG should be controlled to its lower bound to minimise H₂ rich gas (though low purity) from being misused as fuel gas. It should be born in mind that minimum LPHG is tied up to header's basic pressure control. This explains why it is required certain valve opening to ensure control capacity, being this minimum directly related to the LPHG lower bound. In Fig. 6 reconciled and optimum LPHG figures are presented. The gap between REC and OPT of LPHG is presented in Fig. 7. The RTO was able to keep LPHG to its lower bound almost at every execution, while the DMC kept it above systematically. In particular, it seems to be worse in period 2 than in period 1. This might be due to higher H₂ production availability, that will always be beaten by HC load increases. That is the case of period 2 from execution 32 to 51 (see Fig. 3) increasing HC loads and consequently LPHG increases as well (see Figs. 6-7). This reasoning explains as well those OPT points well above the lower

bound (period 2, Fig. 6), which means that the best HC loads possible required more LPHG. Operation in period 1 is much tighter in H₂ terms and therefore the RTO proposes operation closer to the lower bound in all executions. It should be born in mind that the RTO worked out its model on flowrates, purities, pressures and temperatures, not valve opening rates. However, the DMC had the opening of the pressure control valve to FGH as CV (representing the LPHG). Therefore, even at the lower bound (minimum opening) actual flowrates vary due to gas composition fluctuations. Hence, a fixed minimum flowrate for LPHG does not ensure actual minimum being only an orientative figure. For instance, in these periods a more sensible lower bound might have been between 150 and 200 %, though the previous analysis is still valid. In fact, the network operated in both periods with a [REC-OPT] gap close to 100%, which suggests that either the OPT was not achievable or LPHG was well over its lower bound. The latter was not the case for the pressure control valve did operate at its lower bound during several executions.

Based on the previous, the problem of how to define the lower bound for the LPHG at the RTO level arises. Should it be a theoretical minimum flowrate or a valve opening? For the validation process was decided to maintain a flowrate, though it should be updated to reflect a sensible figure of the LPHG. Therefore, using charts as Figs. 6-7 these more sensible figures could be estimated, although they should be revised systematically in order to account for changes in gas compositions. Results from updated lower bounds were not available at the moment of writing this work, that is why they were not presented.

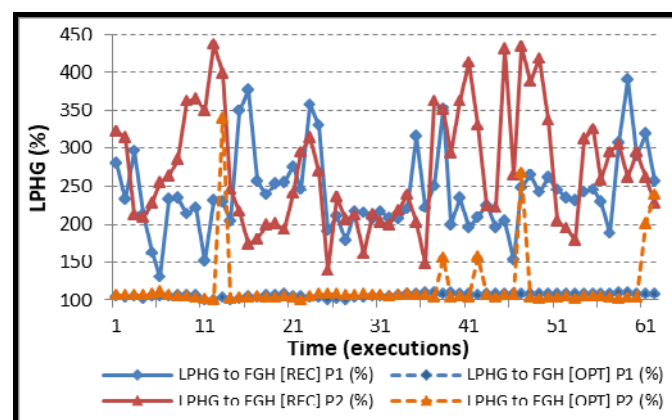


Fig. 6. Low purity header gas purge (REC and OPT) for periods 1 and 2 (P1-2).

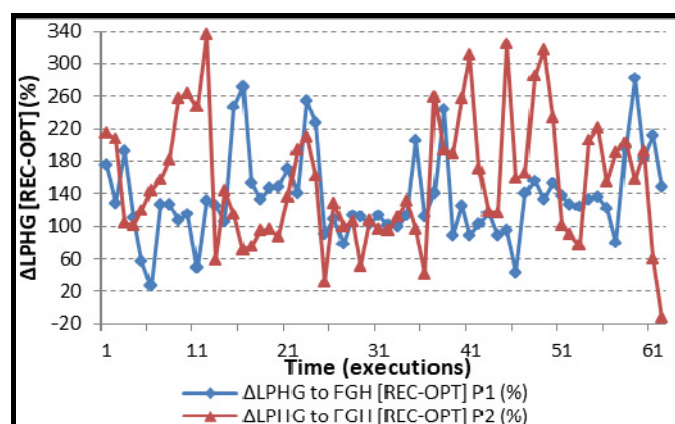


Fig. 7. REC - OPT gap of low purity header gas purge (Δ LPHG) of period 1 and 2 (P1-2).

3.3 Membranes utilisation

According to the previous points (headings 3.1 and 3.2), and the fact that the membranes were not considered by the DMC (see Table 1), is important to analyse REC and OPT figures of the membranes (Z1 and Z2). It must be born in mind that Z1 provides a H_2 purity increase of about 20% and Z2 about 4%. At the same time, Z2 is typically more time on duty than Z1 without any particular reason (see Figs. 8-9). Moreover, Z1 was typically in operation when H_2 scarcity was notorious, e.g.: period 1 (see Figs. 8-9). The rest of the time only Z2 was in service, regardless of any other considerations, e.g.: period 2 (see Figs. 8-9). In fact, Z1 presents mostly negative [REC-OPT] gaps, see Fig. 10, meaning that it was subtilised according to the RTO, though it was off duty (see Fig. 8). For instance, in this case the RTO suggested the operation of Z1 to minimise giveaways in the purification membranes, which would have been determinant to aid the operators in their decision making process. Since the operation of membranes was not controlled automatically it was necessary an operator intervention to decide whether to run them or not. According to what our team surveyed, there was not a clear guideline for operators on this subject. Therefore, it was basically run only when H_2 production was constrained, which coincides with Fig. 8 trends.

Conversely, Z2 ran at all times, though the optimal would have been shutting it down (Fig. 9). This explains the positive figures of [REC-OPT] gap shown in Fig. 10. Bearing this in mind, it seems important to aid operators in their decision of which combination of membranes (Z1, Z2, both or none) is suggested for any actual process situation. For example, the RTO was useful for realising how the optimal H_2 distribution would look like, complementing the DMC control. It would have aided operators in their decisions regarding the H_2 network management. Particularly, it might have been useful for deciding on the membranes operation, as discussed before.

It should be noticed that, membranes were not explicitly represented in the RTO's cost function. However, they have

an implicit cost due to their required purge to FGH (represented as PG in 2).

Therefore, the RTO sorts out whether to run a membrane or not depending on a trade-off between: increasing H_2 purity in the LPH at the cost of increasing purge to FGH, and increasing H_2 production or cutting down HC loads. Thus, when the H_2 production constraint is already active, HC loads definitely pay-off and the membranes become clearly beneficial to the process economy. However, when the H_2 production is not constrained, and HC loads are already at their maximum, H_2 purity increase may not pay-off due to the cost of misusing H_2 rich gases against H_2 production costs.

3.4 Limitations

A complementary analysis based on Lagrange multipliers would allow a better understanding of the RTO solutions. For instance, it may aid operators in their decisions whenever they face constraints violations in the actual process. Lagrange multipliers could be used as a quantitative criterion of the impact in the process economy of such violations. Although those from the RTO were incorporated recently in the plant information system, they were not available at the moment of collecting data for this study. Hence, is highly suggested to incorporate these into the analysis and discuss how to pass it on to the operators effectively and support their decision-making process.

In addition, the DMC has steady-state constraints on its optimisation layer, though those cannot ensure constraints violations along transitions. Moreover, any application to be deployed should be compatible with the DMC in order to be actually used by operators. Given this framework, path constraints may be addressed by applying predictive simulation. Therefore, operators would be able to consider RTO set points and check with a simulation how the system dynamics reach new steady states. Certainly, this approach requires specific studies and should be considered in future works.

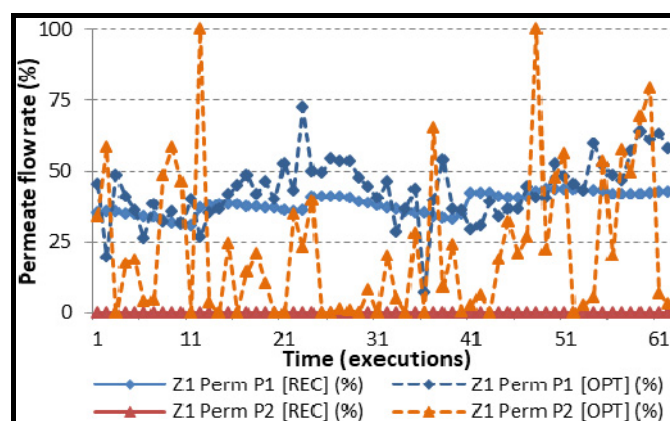


Fig. 8. Purification membrane Z1 REC and OPT for periods 1 and 2 (P1-2).

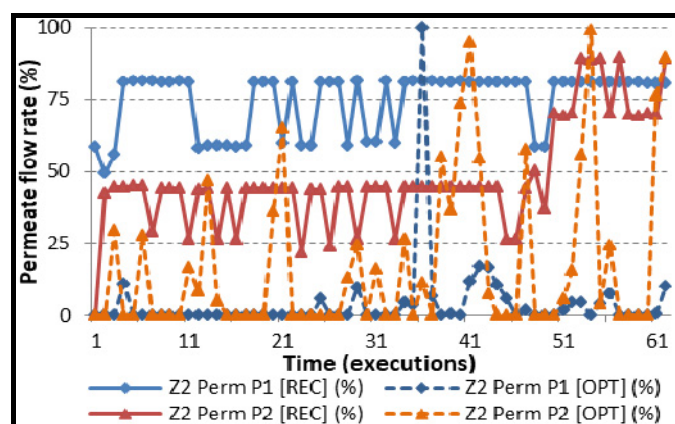


Fig. 9. Purification membrane Z2 REC and OPT for periods 1 and 2 (P1-2).

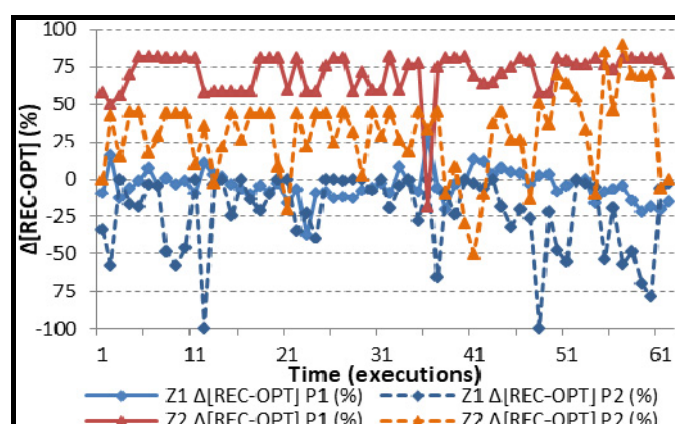


Fig. 10. REC - OPT gap of Z1-2 ($\Delta[\text{REC-OPT}]$) of period 1 and 2 (P1-2).

4. CONCLUSIONS

The validation process of a prototype RTO of a refinery H_2 network was presented, and analysed focusing on its utility as a decision support tool for operators. In particular, the analysis compared actual reconciled data, of two representative operation periods, against RTO figures for shortlisted variables. H_2 production, HC REI, LPHG and membranes permeate were deemed the most important variables at network level.

The RTO successfully managed scenarios of H_2 scarcity, achieving minimum LPHG and maximum HC loads. In particular, it provided valuable information for operators to decide whether each membrane should be in service or not. Mainly due to the lack of automatic operation of the membranes, and their absence in the DMC model, the RTO arrived to less expensive process conditions in both periods (P1-2). In overall, the validation process was successful and the RTO information proved usefulness for the decision support of operators.

Limitations of the approach and future work directions were discussed as well, such as the most appropriate LPHG lower

bound, incorporation of Lagrange multipliers to the analysis and how to deal with transition states.

5. ACKNOWLEDGEMENTS

Financial support is gratefully acknowledged from the Marie Curie Horizon 2020 EID-ITN project "PROcess NeTwork Optimization for efficient and sustainable operation of Europe's process industries taking machinery condition and process performance into account – PRONTO", Grant agreement No 675215. The authors are thankful to the Spanish Government support with project INOPTCON (MINECO/FEDER DPI2015-70975-P), as well as Petronor and its management for supporting this study.

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