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Implementation of RTO in a large hydrogen network considering uncertainty

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Abstract: This paper first describes the problems associated to the implementation of a RTO system to optimize the operation of a large scale hydrogen network of an oil refinery, and then explores how to incorporate explicitly in the decision making process the uncertain factors associated to its operation in order to improve the management of the network made by technical staff.

Keywords: Process optimization, Hydrogen networks, Real-time optimization, Two-stage stochastic optimization, CVaR

1. INTRODUCTION

Process optimization is one key component in order to achieve the level of efficiency that is required today in process plants. Among the many different ways in which optimization can be used in the management and control of a plant, operating it in the best possible way is one of the most challenging and, at the same time, rewarding problems because of its complexity and impact on the efficiency and results of the company.

Decisions about the production and operation of a process plant are organized hierarchically in a set of layers, as in Fig.1. Darby et al. (2011). This is a simplified schematic not covering other important features, but represents the main elements for the purpose of the paper.

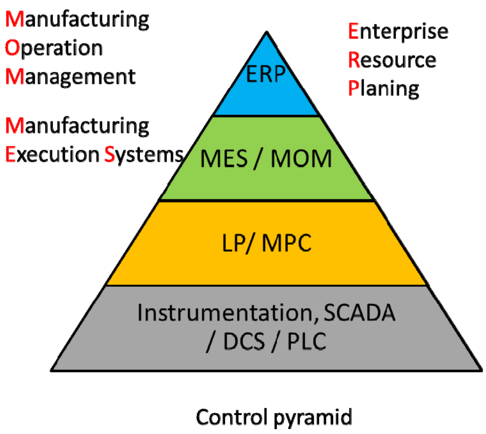

Fig. 1. Hierarchical decision layers for process control and operation

Basic control is in charge of keeping safety and stability of the plant under control, implementing the control room operators' or upper layers decisions. The Model Predictive Control (MPC) layer targets improving control by considering the interactions, disturbances and operation constraints associated to process units or small plants. Within the MES/MOM layer, the main element for the purpose of this paper is Real Time Optimization (RTO), which aims at computing the operation points of the process units that optimize production according to a certain criterion while satisfying process constraints. A RTO system normally uses large non-linear models covering a whole plant, section or complex process unit maximizing or minimizing a target limited to that scope. At this point, besides the "local" optimization of process units, RTO has to consider the interactions between the different plants and relevant process units that compose a process factory. If not computed by the RTO layer, the variables associated to the global functioning are normally decided by the plant managers according to experience or heuristics, but these decisions are difficult to take due to the complexity of the problem, lack of information or adequate models, affecting negatively the plant performance.

Of course, at the ERP level, the production planning tools may generate global targets for the different sections of a plant, but these are “averaged” targets to be taken as references for several days or weeks, that are not useful for real-time operation where, due to the variability of products, external disturbances, dynamic decisions are required in order to avoid creating bottlenecks, violating constraints or risking the safe operation of the plant, while being as close as possible to the optimum operating point of the whole plant.

The standard architecture of Fig 1, with an RTO layer that uses non-linear steady-state models to generate fix targets for the MPC for periods of the order of hours does not manage properly the dynamic aspects above mentioned. Alternatively, the RTO and MPC layers can be combined in an economic MPC or optimal dynamic operation problem as in Engell (2007) and Gonzalez, Zamarreño, de Prada (2001). This approach solves the inconsistency problem between layers that may appear due to the use of different models in RTO and MPC, and it is well stablished for continuous processes, but requires solving large-scale dynamic optimization problems in long computation times in order to allow for real-time implementation, which may be a significant obstacle for its implementation.

This paper proposes another way of considering the joint operation of large-scale RTO with MPC, and illustrates the methodology in a case study corresponding to the hydrogen network of an oil refinery involving the joint operation of 18 plants, discussing its implementation and results. In addition, the paper expands previous results (de Prada et al., 2017) analyzing the convenience of expanding the optimization with the explicit consideration of the uncertainty associated to some important variables, studying two alternative formulations based on two-stage stochastic optimization.

The paper is organized as follows. After the introduction, section 2 describes the hydrogen network under consideration and the formulation of the optimization problem. Then, section 3 presents the architecture of the system implemented in the refinery and discuss some results. Next, section 4 is devoted to formulate and discuss the stochastic problem considering two possible aims, one of which includes risk. The paper ends with conclusions and references sections.

2. HYDROGEN NETWORK

2.1 Process description

Hydrogen is used in oil refineries with two main purposes: converting heavy hydrocarbons into lighter ones in order to improve the profitability of the business, and removing sulphur from hydrocarbons in order to comply with environmental regulations. Because of that, it has become one key utility in the operation of the refineries. Hydrogen is obtained either from an external supplier or internally from steam reforming plants, as well as a sub-product from the platformer plants used to increase the octane number of gasolines and then it is distributed to the consumer plants through pipelines forming a complex network. A general overview of hydrogen supply chain for general purposes is explored by Ochoa, Zondervan (2018).

In the particular refinery under consideration the network involves 18 plants: two producers of fresh hydrogen, two platformer plants and 14 consumer plants, most of them hydrodesulphurizers connected by means of several headers that operate at different pressures and hydrogen purities as in Fig 2. Notice that a consumer plant can be fed from different sources.

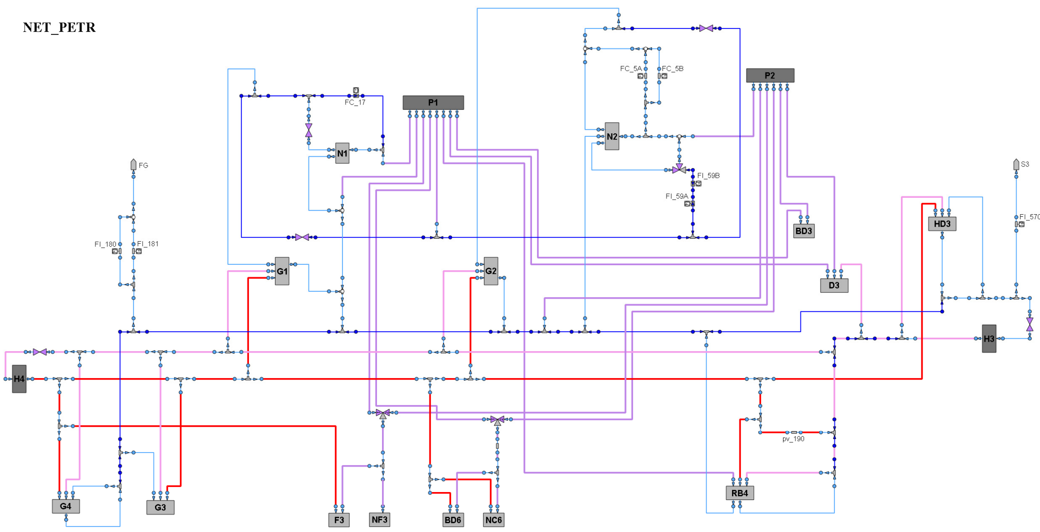

Fig. 2. Schematic of the hydrogen network with producer (grey boxes) and consumer (light green boxes) plants connected by several headers, among them H4 (red), H3 (light purple) and LPH (blue).

A simplified schematic of a typical hydrodesulphuration plant can be seen in Fig 3. The hydrocarbon feed is mixed with hydrogen coming from different sources to be treated in endothermic reactors. One important aspect of the operation is the fact that preserving catalyst life in the reactors requires to supply always a certain excess of hydrogen. Since hydrogen is a product that is very difficult to store and the plants have variable hydrogen demand according to the type and flow of the hydrocarbons being treated, the producer plants always generate more hydrogen than what is consumed in order to guarantee that enough hydrogen is available under any circumstance. This will avoid damaging the expensive catalysers, but an overall excess hydrogen is sent to the refinery fuel-gas network to be burnt in furnaces. As hydrogen is expensive to produce, a good management of the network should coordinate the operation of all plants, matching demand and production in order to minimize losses of hydrogen to fuel-gas.

At the same time, as can be seen in Fig 3, within the consumer plants some separation units try to recover the excess hydrogen, which is partly recycled with a compressor, purified by the use of membranes and recycled, or partly sent to the fuel-gas FG network or low-purity header CBP in order to prevent accumulation of impurities.

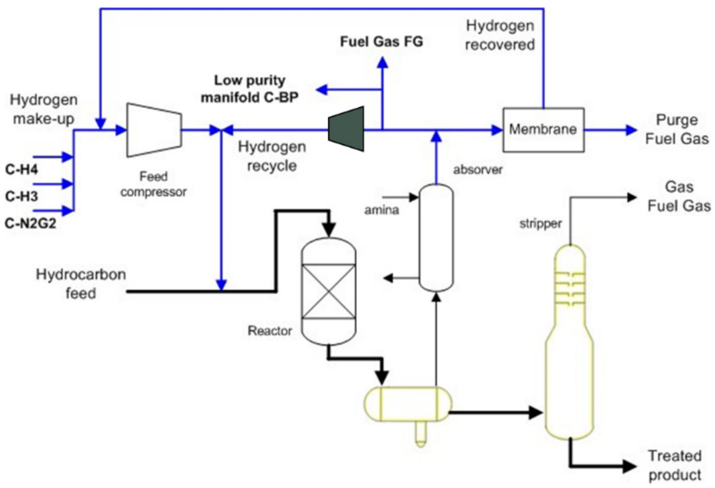

Fig 3. Simplified schematic of a hydrodesulphuration plant

Another key point related to the operation of the reactors is purity. Catalytic reactions require hydrogen to be supplied with a certain minimum hydrogen purity. The hydrogen that is recovered from the separation units has a lower purity than the one that feeds the reactors, but its purity can be increased using membranes or, after being sent to a Low Purity Header (CBP), reused in other plants either directly or mixed with fresh hydrogen to increase its purity. As a result, the hydrogen network operates with several headers at different purities and pressures as represented in the simplified schematic of Fig 4, which displays two producer units with their corresponding headers, supplying hydrogen to three consumer plants that deliver or consume recycled hydrogen from the CBP, and may also send hydrogen to the FG network.

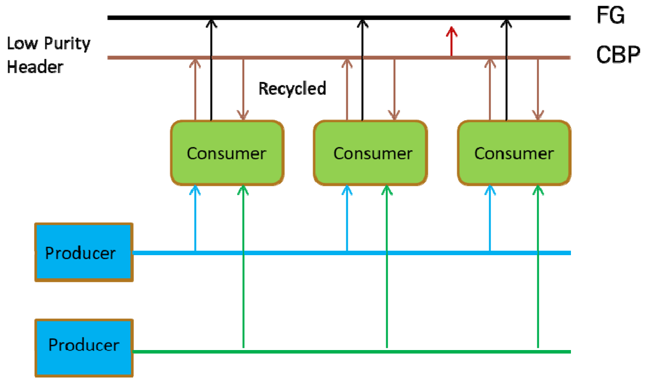

Fig 4. Schematic showing the different types of headers found in a hydrogen network:, fresh hydrogen (blue and green), Low purity header (CBP brown) Fuel gas network FG, black)

Proper management of the network requires deciding in real time, according to the hydrogen demands from the reactors and variable hydrogen flows generated by the platformer plants, how much fresh hydrogen should be produced by each producer plant, and how to distribute the hydrogen through the network and internally in the consumer plants so that the losses to FG, or in general costs, are minimized. In addition, the operation of the network has to consider as the most important economic target the maximization of the hydrocarbon loads processed in the hydrodesulphurization plants, which may be limited by the hydrogen available and the production aims stablished by the planning of the refinery for the period under consideration. Notice that reducing losses of hydrogen to FG may increase the hydrocarbon processing if hydrogen is the limiting factor, which provides additional value to the optimal management of the network. Of course, optimal decisions must satisfy all process constrains imposed by the equipment, operation, safety, targets or quality.

2.2 Models and data reconciliation

Optimization of the complex system requires proper network and plant models validated against process data. One of the main obstacles in developing these models is the lack of reliable information about many streams and compositions besides the nature of hydrogen. Most of the hydrogen flow measurements are volumetric ones that must be compensated using pressure, temperature and molecular weight of the stream to obtain mass flows. Nevertheless, hydrogen purity measurements are not always available and, even when it is measured, the molecular weight of the stream is unknown and unreliable. This is due to the fact that the gas stream contains impurities (light ends) of unknown and changing molecular weight much larger than the one of hydrogen, which is only 2. E.g., a stream with purity 90%, where one half of the impurities change composition, for instance from methane to propane, can change the molecular weight of the stream in 41%. Notice that besides flows and compositions, other important variables, such as hydrogen demand in the reactors, are not measured and change over time with the types of hydrocarbons being processed.

This means that, before any optimization can be performed, a procedure to obtain reliable information from the plant using the plant measurements should be implemented. Data reconciliation can be used for this purpose as it offers a way of estimating the values of all variables and model parameters coherent with a process model and as close as possible to the measurements. Data reconciliation is formulated as a large optimization problem searching for the values of variables and parameters that satisfy the model equations and constraints and that, simultaneously, minimize a function of the deviations (e) between model and measurements, properly normalized.

In our case study, a first principles model of the hydrogen behavior in the network and associated plants was available from previous work (Sarabia et al. 2012), (Gomez, 2016). It is based on mass balances of hydrogen and light ends (considered as a single pseudo-component) in all nodes of the network as in the pipes and units as in (1), where *F* stands for stream flows, *X* are hydrogen purities and *PM* refers to molecular weights:

$$\sum_{i,sale} F_{N,i} = \sum_{j,entra} F_{N,j}$$
$$X^{H2} \sum_{i,sale} F_{N,i} = \sum_{j,entra} X_j^{H2} F_{N,j}$$
$$PM \sum_{i,sale} F_{N,i} = \sum_{j,entra} PM_j F_{N,j}$$
$$100 PM_k = PM^{H2} X_k^{H2} + (100 - X_k^{H2}) PM_k^I \qquad (1)$$

In addition, the model incorporates other equations for compressors, membranes, separation units (including a solubility model), etc., some of which are reduced order models fitted to experimental data or with some adjustable parameters. Taking into account the much faster dynamics of the hydrogen compared to the dynamics of the reactors, the hydrogen distribution model is static and contains flows, purities, molecular weights of hydrogen and light ends of all streams and hydrogen consumption in the reactors as main variables.

The data reconciliation problem requires a certain degree of redundancy in the measurements and is formulated as the following NLP problem:

$$\min_{\{F_i, X_i, MW_i, \varepsilon_i, p_i\}} \sum_{j \in M} \alpha_j c^2 \left[\frac{|e_j|}{c} - \log\left(1 + \frac{|e_j|}{c}\right) \right] + \sum \alpha_i \varepsilon_i^2 + \sum \alpha_k R_k \qquad (2a)$$

s.t.

model equations

operational and range constraints

$$F_{i,\min} - \varepsilon_{Fi} \le F_i \le F_{i,\max} + \varepsilon_{Fi} \quad \varepsilon_{Fi} \ge 0$$
$$X_{i,\min} - \varepsilon_{Xi} \le X_i \le X_{i,\max} + \varepsilon_{Xi} \quad \varepsilon_{Xi} \ge 0$$
$$MW_{i,\min}^{imp} - \varepsilon_{Wi} \le MW_i^{imp} \le MW_{i,\max}^{imp} + \varepsilon_{Wi} \quad \varepsilon_{Wi} \ge 0$$

(2b)

$$\text{where} \quad \begin{array}{l} e_j = \eta_j (F_j - \beta_j F_{i,mea}) \\ e_j = \eta_j (X_j - X_{j,mea}) \end{array} \quad \beta_j = \sqrt{\frac{T_d + 273}{(P_d + 1) MW_j}} \sqrt{\frac{(P_j + 1) MW_d}{T_j + 273}}$$

The above NLP minimizes the function (2a) of the errors e_j between the measured flows $F_{j,\ mea}$ and purities $X_{j,\ mea}$, and the same magnitudes computed with the model under the links imposed by the model and other operational and range constraints. The coefficients β represent the compensation factors, and the variables ε are slack variables to ensure feasibility in the range constraints, while *R's* are regularization terms to avoid sharp changes. Index *i* expands to all streams while index j refers to the measurements. Notice that instead of the common sum of squares of the errors, a robust M-estimator as the Fair function has been used, which is similar in shape to the sum of squared errors for small values of the error but grows slower for larger ones limiting the effect of gross errors in the data.

The data reconciliation problem is a large-scale Non-Linear Programming (NLP) that is formulated and solved with a simultaneous approach in the General Algebraic Modeling System (GAMS) using the Interior Point Optimizer (IPOPT) as the optimization algorithm. The implementation involves more than 4400 variables and 4700 equality and inequality constraints. It takes less than five Central Processing Unit (CPU) minutes in a PC with i7 processor and 8 Gb RAM, giving robust results against gross errors and helping to detect faulty instruments.

2.3 Network RTO

Once a sensible model and reliable corrected measurements are available, one can formulate the network optimization problem as finding the production and redistribution of H_2 in the network and the value of the hydrocarbon loads to the consumer plants that maximizes the value associated to the loads taking into account the cost of generating hydrogen, which corresponds to the cost function:

$$\max J = \sum_i \mathrm{p}_{\mathrm{HCi}} HC_i - \sum_j \mathrm{p}_{\mathrm{Hi}} F_{Hi} - \sum_k \mathrm{p}_{\mathrm{Rk}} R_k \tag{3}$$

where p represent prices HC are hydrocarbon loads, F fresh hydrogen and R deals with the compression cost of the recycled one.

This function is maximized respecting all constraints and without changing the way the reactors are operated, that is:

- Maintaining the current ratio of consumption of H_2, light gases generation and their properties (purity and molecular weight) in each reactor
- Maintaining the ratios in purge flow from low pressure separators and its properties (purity and molecular weight)

These values are estimated every two hours from the data reconciliation step and are expected to be the same in the (near) future, if there is no change in hydrocarbon feed quality.

In the optimization, besides the network model, the main constraints refer to the process operation (ranges, H_2/HC, compressors capacity and maximum purity,…) and refinery planning specifications. Main decision variables include production of fresh hydrogen, feeds to consumer plants, hydrogen flows and recirculation, purges, purities and membranes operation.

The RTO is solved as an NLP problem in the GAMS system. It involves nearly 2000 variables and more than 1800 equality and inequality constraints and is solved with a simultaneous approach and the IPOPT algorithm in less than one minute CPU time.

3. SYSTEM ARCHITECTURE FOR OPTIMIZATION

The data reconciliation and network RTO are implemented according to the architecture displayed in Fig 5.

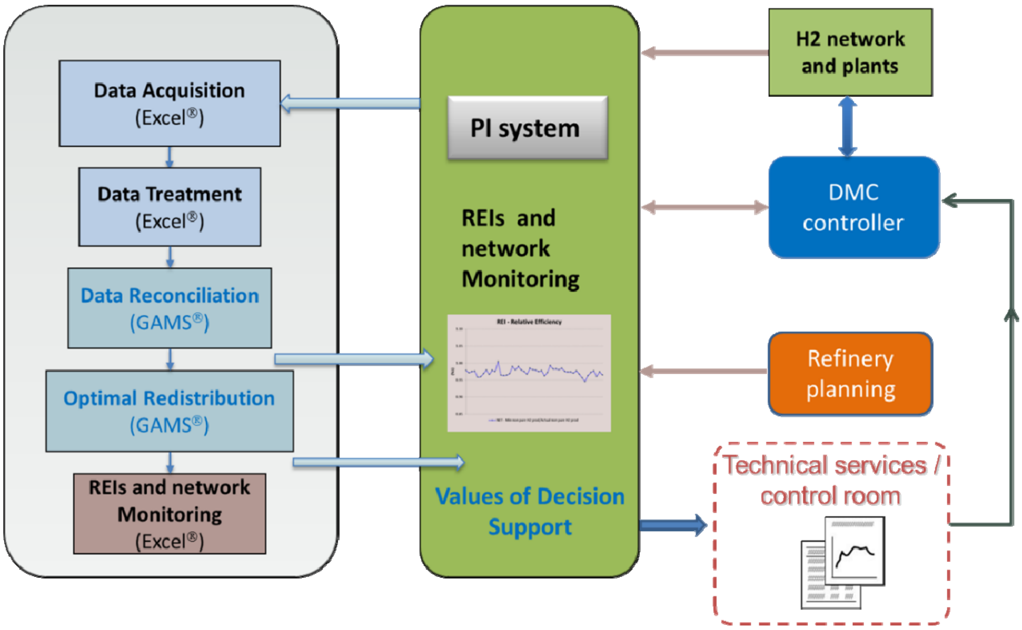

Fig 5. Schematic of the system's architecture displaying the DR-RTO module on the left hand side, the PI system in the center and process and other control and planning elements on the right hand side.

Data and measurements from the hydrogen network are stored regularly in the real-time information system of the refinery (Osi-PI). Values of each of them are read every two hours from the PI system to be processed in the DR-RTO application which resides in a dedicated PC. The application is composed of several modules as shown in the left hand side of Fig 5. The data acquisition module reads 171 flows and 18 purity measurements, plus other variables and configuration parameters from the PI (temperatures, pressures, valve openings, etc.) totaling around 1000 variables, averaging them in two-hour periods to smooth the effects of transients and disturbances. Data treatment is a critical component that contains a set of rules dedicated to detect faults and information inconsistences in the raw data and decides which options, variable ranges, etc. are the most adequate ones in the mathematical formulation of the problems. In addition, this module detects when a plant is out of service or a hydrogen header has modified its connectivity, such that its associated equations should be removed or changed in the network models. To implement this variable structure operation, the models are formulated as a superstructure that includes binary variables such that, according to the analysis of the data treatment module, the model can be adapted automatically to the state and configuration of the plants and headers.

Then, the treated data and constraints are sent to the data reconciliation module that solves the corresponding optimization problem and provides updated and reliable information and parameters to the network optimization module (named as Optimal Redistribution in Fig 5). Finally, the information from the data reconciliation (DR) and the network optimization are used to compute some Resource Efficiency Indicators (REIs), and all of them are sent back to the PI refinery information system, where they are available to all potential users.

A first benefit of the system is providing improved process information and, in particular:

- an indication of possible faulty instruments
- reliable balances of hydrogen
- values for unmeasured quantities (purities, molecular weights, hydrogen consumption, …) not available previously
- data for computing REIs that allow better monitoring of the operation of the network

Regarding the implementation of the solutions of the optimizer, ideally, the optimal values calculated should be sent as set-points to the network control system, either directly to the flow controllers or following the traditional architecture as in Fig 1. Nevertheless, the static nature of the RTO and the low frequency of its execution bring several problems as the implementation of the optimal values has to be applied to the process taking into account the time evolution of variables. In particular, HC loads and hydrogen production have to be changed dynamically at a higher frequency to balance hydrogen production and consumption. In the same way, due to the presence of disturbances, changing aims, etc., constraints' fulfilment requires dynamic actions to be performed at a higher rate, and changes in hydrogen flows may interact among them so that a proper implementation of the RTO solution would require multivariable control to take care of the interactions. Because of that, a different approach has been considered.

3.1 Implementing Network Optimization in real-time

A direct way of incorporating dynamics into the system, solving simultaneously the problem of possible inconsistencies between the non-linear RTO model and the linear one typically used in the MPC layer, is to formulate a single integrated dynamic optimization problem as mentioned in the introduction. Nevertheless, it is not realistic maintaining and operating in real-time a dynamic data reconciliation and dynamic RTO system involving 18 plants due to its large scale. A different alternative, somewhere in the middle between sending set-points from a RTO to a MPC and direct dynamic optimization with economic aim, was considered and implemented in the refinery. For implementation, it takes advantage of the fact that some commercial MPCs, e.g. DMC+, are actually composed of two layers: a Dynamic Matrix Controller (DMC) to compute control actions, and a local optimizer on top that, using Linear Programming (LP) and sharing the same linear dynamic models as the DMC, computes on-line targets for the multivariable controller minimizing a user defined economic function.

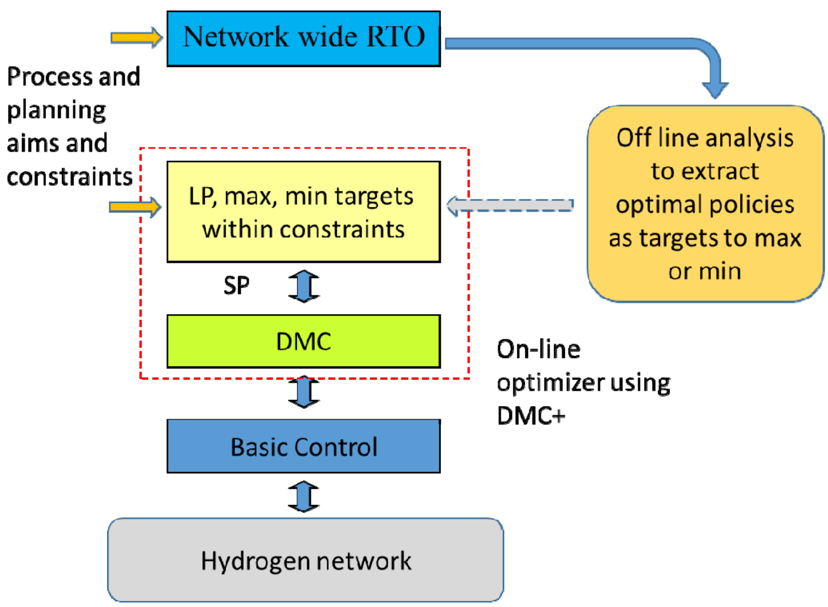

Fig 6. Schematic representing the methodology for on-line implementation of RTO policies.

The methodology is represented in Fig 6, and basically consists on analyzing the network RTO solutions and extract from them optimal *policies* that are consistently recommended by the optimizer. This means understanding the logic behind the solutions and identifying variables that should be maximized or minimized, but their specific value depending on the process constraints or planning specification. Then, these policies are implemented as targets (variables) to maximize or minimize in the LP layer of the DMC as linear combinations with weights reflecting priorities and costs. The LP determines the optimal values compatible with the actual process model, process state and constraints and generates the corresponding set points to the DMC controller, which, finally, taking into account systems dynamics and interactions, will compute current and future hydrogen and hydrocarbon set points to be given to the individual low level flow controllers of the DCS of the control room.

In the case considered, the optimal policies identified were:

- Losses from the HP separators of a plant to fuel gas, required to avoid light ends accumulation, should be made at the lowest hydrogen purity compatible with the one required at the reactor input and the H_2/HC minimum ratio, but the CBP purity should be maximize to increase hydrogen re-use.
- The hydrogen unbalance in the network, that is, hydrogen generated minus hydrogen consumed in the reactors, reflects in the CBP pressure, so losses to fuel gas from this header should be minimized with a minimum to guarantee unsaturated operation of the pressure controller.
- Maximization of the hydrocarbon load to the consumer plants, which is the most important target, and can be made until either maximum hydrogen capacity is reached or another technical constraint is faced.
- Sending higher purity hydrogen (H4) to lower purity header (CBP) should be minimized as purity degrades.

The system was implemented in the refinery shown in Fig 5, but with the DMC controller covering only the six most important plants from the hydrogen use point of view as a compromise between maintenance and development costs and potential benefits as in Fig 7.

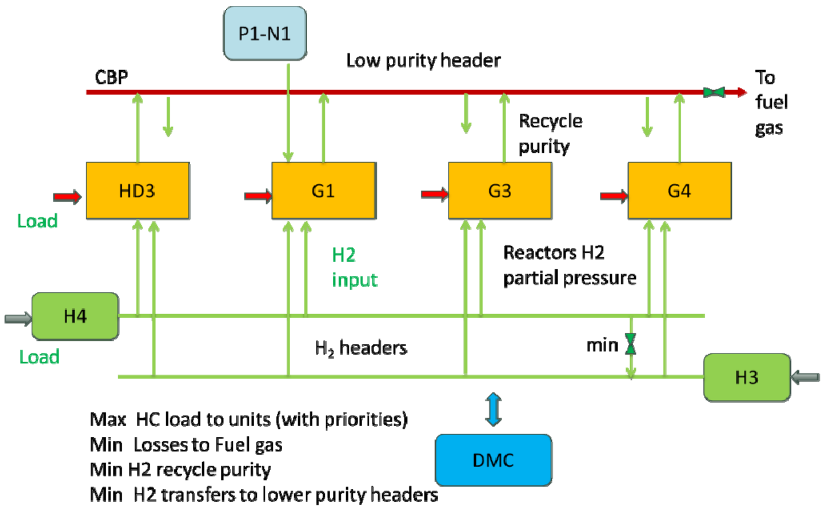

Fig 7. Diagram of the DMC controlling the operation of two hydrogen producers H3 and H4 and four consumers G1, G3, G4 and HD3, with the main controlled hydrogen flows and HC loads

The DMC controller manages two hydrogen producers (H3, H4) and four consumer plants (G1, G3, G4, HDS) and was developed and implemented by the refinery team. It is based on linear models obtained by identification using data from step-tests that forms a dynamic matrix involving 12 manipulated variables and 29 controlled ones. The main manipulated variables refer to the set points of hydrocarbon loads to the consumer units, fresh hydrogen production, hydrogen feed to the consumers from the high purity collector, and supply of hydrogen from one of the platformer plants. The main controlled variables are hydrogen partial pressure in the reactors of the consumer plants, losses to fuel gas from the Low Purity Header (valve opening), recycle purity and HP losses to FG from some plants, hydrocarbon loads and valve openings to avoid control saturation.

The cost function in the LP layer combines four targets that together synthesize the solution of the RTO:

- Maximize hydrocarbon loads to the consumer plants
- Minimize losses from the CBP to FG
- Minimize hydrogen purity in the recycles of the consumer plants
- Minimize hydrogen transfers from higher to lower purity headers

The corresponding variables are linked to the manipulated variables through the linear process model, so that the optimization problem is linear and can be solved in a short time. The LP / DMC runs with a sampling time of a minute giving consistent results for many months. In parallel, the network RTO is executed every two hours being operated as a DSS for the whole network and allowing the supervision of the DMC application. As an example of results, Fig 8 displays the total optimal and actual hydrocarbon load to the HDS plants for a period of nine days, showing good performance.

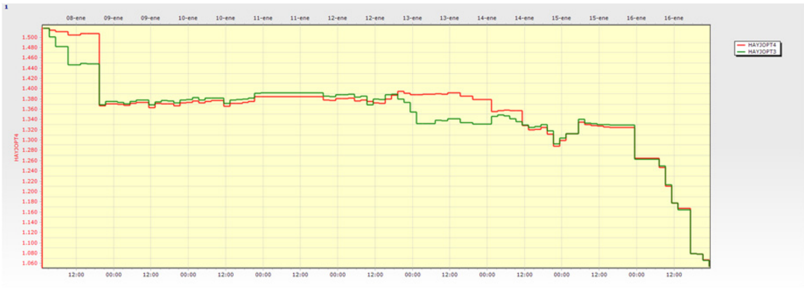

Fig 8. Evolution of the optimum total hydrocarbon load and actual one for a period of nine days

4. TWO-STAGE STOCHASTIC (TSS) OPTIMIZATION

In Fig 8, we can see that the optimal conditions change significantly over time. In fact, the refinery is subjected to potentially large changes every two to three days when it receives new crude oil from ships, not to mention new production targets imposed by market demands.

Changes in the crude oil reflect in changes in the hydrogen consumption of the reactors of the HDS plants that are difficult to predict, creating transients where the performance of the network may suffer degradation. One may wonder if incorporating this uncertainty explicitly in the decision making process would improve significantly the results obtained.

At the RTO level, this is done updating the model and network information at regular intervals by means of data reconciliation. Nevertheless, it is well known that, even with data reconciliation, if the model has structural errors the optimum computed with the model may not correspond to the real process optimum. Alternatively, we can consider different possible values of the uncertain variables and optimize considering the worst case, following a robust optimization approach (Ben-Tal and Nemirovski, 2002). This option chooses the values of the decision variables that guarantee fulfilment of all constraints in all scenarios, but provides very conservative solutions as they are fitted to the worse case. A better approach may be multi-stage stochastic optimization which takes into account that some decisions that influence the future behavior of the process has to be made at current time without knowing the value of the uncertain variables but, in the future, new information can be available that reveals the value of the uncertainty, so that particular correction actions can be made in the future according to the specific scenario that may take place.

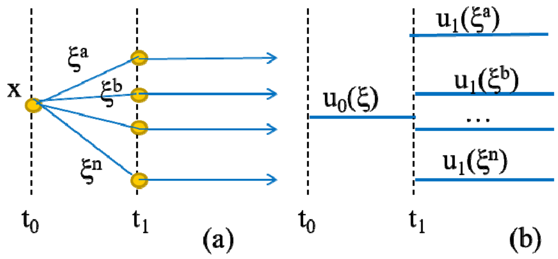

Fig 9. Schematic of the main concepts behind two-stage stochastic optimization and scenario tree representation.

The concept is illustrated in Fig 9, where a scenario tree is represented for a two-stage stochastic model. On the left hand side (a) the system has a state x at time t_0 and a decision u_0 (with some variables known as first-stage ones) has to be made considering all possible values ξ_i of the uncertainty, a scenario is defined as the arc between nodes. After applying u_0, the system will evolve in t_1 to different states depending on the specific value of ξ_i, but if this value were know at t_1, we could compute a specific optimal decision $u_1(\xi_i)$ for each value of ξ_i in the period of time starting at t_1 for the remaining variables (recourse variables), as in Fig 9 b. This section studies the value of the stochastic approach applied to the hydrogen network in order to evaluate the interest of its implementation.

4.1 Formulation of the TSS problem

Main elements in the formulation of the optimal management of the hydrogen network as a two-stage stochastic optimization problem are: the identification of the uncertainty source, the scenarios definition with their likelihood of realization, and selection of meaningful first and second stage variables. Regarding the objective function, the simplest approach is to formulate the deterministic equivalent problem (DEP) of the minimization as in (4). A detailed discussion on alternative formulations of TSS problem could be found in Birge and Louveaux (2010).

$$\min_{u_F, u_{S(\xi)}} J_F(u_F) + \mathbb{E}\{J_S(u_F, u_S(\xi), x_S(\xi))\} \quad \forall \xi \in \Xi$$
$$h_F(x_F, u_F) = 0, \qquad g_F(x_F, u_F) \leq 0$$
$$h_S(x_F, u_F, u_S(\xi), x_S(\xi)) = 0, \qquad g_S(x_F, u_F, x_S(\xi), u_S(\xi)) \leq 0 \tag{4}$$

where: $(\cdot)_F$ refers to variables or functions in the first stage and $(\cdot)_S$ denotes the ones in the second stage, while the decision variables are denoted as u and the remaining variables as x. The uncertainty is represented by the parameters ξ_i that can take values within a set Ξ according to a certain probability distribution. Normally this set is sampled and only a finite number ξ_i , i = 1,2,3,…,n of elements is considered, which constitute the scenarios that will represent the uncertainty. In the objective function the sum over all scenarios i represents the expected value of the objective function over the second stage variables.

The cost function is composed of two terms: The first one, J_F, is the cost in the first stage which depends on the first stage decisions u_F. These are decisions that are taken and applied at current time without knowing the particular realization of the uncertainty ξ and will be maintained over the time horizon covered by the optimization problem. Consequently, they are the same for all values of ξ_i. Nevertheless, we can correct the effects of the u_F decisions once the value of the ξ_i parameters are revealed, using the recourse variables $u_S(\xi)$ that take a particular value for each realization of the uncertainty (ξ_i). The second term of the cost the weigthed summation over all the scenarios with corresponding probabilities π_i, represents the effect of these second stage corrections on the total value of the cost function, which also depend on the u_F decisions.

The variables of the problem have to satisfy the constraints imposed by the model *h(.)* and additional inequality constraints *g(.)* in every stage for all possible scenarios considered (n). In (4), the corresponding equations, that depend on the stochastic parameter ξ, should be interpreted as being fulfilled with probability one.

4.1.1 Uncertainty source description

Hydrogen gas in a refinery is basically a utility, for it is demanded and consumed in process units and it should be enough to satisfy the process requirements at all times. The deterministic problem tackles the optimal hydrogen management problem assuming that hydrogen demand of each plant is to be calculated exactly using the results of the DR problem. However, this concept does not hold when the refinery is facing crude oil changes, which typically imply hydrogen demand swings as well. In these situations, predictions of hydrogen demand at the plant level are usually inaccurate due to the fact that hydrocarbon cuts properties may be estimated with large errors, which make them the main source of uncertainty. Fig 10 presents a simplified oil refinery schematic representing the different intermediate cuts fed to hydrogen consumer units (i.e.: HDS, HDT, HDC), which will be impacted by changes in the hydrocarbon properties and ultimately lead to hydrogen demand changes. Therefore, a scenario tree representation is applicable in this context as seen in Fig. 9. In addition, in most cases hydrogen demand affect all consumers in the same direction (i.e.: increase or decrease) as a consequence being fed by a unique crude oil source (see Fig. 10). It must be present that refinery hydrogen networks are very specific due to all the features described before. Other gas networks cases studies available in literature, such as the one by Li, Tomasgard and Barton (2017) for natural gas networks, may differ in most of the assumptions and features, though the stochastic approach still holds in all.

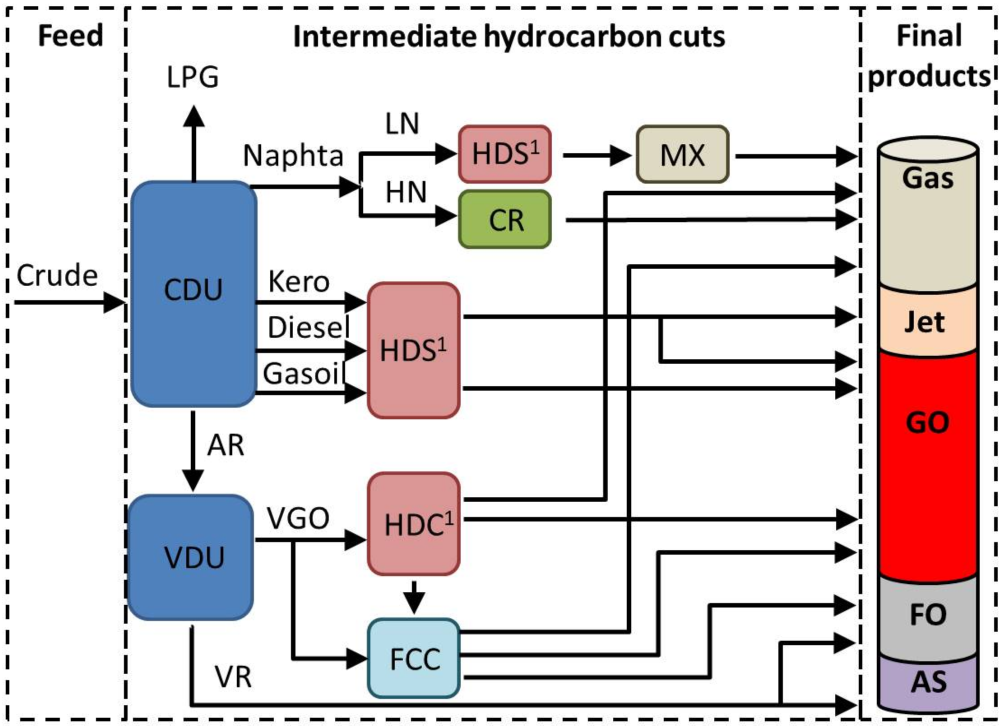

Fig. 10 – Simplified schematic of an oil refinery, identifying the main intermediate cuts fed to process units. CDU – Crude distillation unit. VDU – Vacuum distillation unit. HDS –

Hydrodesulphurization unit. HDC – Heavy oil desulphurization unit. FCC – Fluidized catalytic cracking. CR – Catalytic reforming. MX – Merox sweetening. LPG – Liquefied petroleum gas. Kero – Kerosene. LN / HN – Light and heavy naphta, respectively. AR – Atmospheric residue. VR – Vacuum residue. Gas – Gasoline. Jet – Aviation jet fuel. GO – Commercial gasoil. FO – Fuel oil. AS – Asphalt. [1] Major hydrogen consumer.

4.1.2 Scenarios definition

Given different potential hydrogen demands at plant level is possible to link those to a probability of occurrence ($\pi(\xi_i)$), which will be revealed only after the first stage decisions are due. Therefore, each scenario is identified with a likelihood of realization of a hydrogen demand at plant level. It should be borne in mind that this idea narrows down the search for first and second stage variables, since the former are not affected by the uncertainty of the scenarios.

4.1.3 First and second stage variables

As a consequence of the network dynamics, explained in section 2, hydrogen production decisions at generation units (i.e.: H3 and H4) precede actual plant demand at consumer units by around two hours. In other words, hydrogen demand at any given time should be met by the hydrogen production rates of the past two hours. However, consumer plants have much faster dynamics and cope with most of the changes in feed quality within minutes. Due to the fact that the uncertainty source is from feed quality, which in turn reflects into hydrogen demand at the plant level, scenarios affect all consumer plant variables and headers. Additionally, hydrogen production has to be set two hours before it is actually demanded. Therefore, in the TSS formulation the first stage variables are all related to the hydrogen production units, H3 and H4. The rest of the network variables are all subjected to scenarios hence defined as recourse or second stage variables.

4.1.4 Problem statement

Given the hydrogen network of an oil refinery, with production and consumption of hydrogen, and hydrocarbons processed in consumer plants. The problem is to determine the hydrogen production rate at time t_0 of each producer, such that plants demands' are satisfied for all possible scenarios, complying with operational restrictions. The objective is to maximize the expected profit of the network operation (5), considering hydrogen production costs and revenues from hydrocarbon processing at all scenarios.

$$\max_{F_{H_2}, HC_i(\xi_i), R_i(\xi_i)} J_F\left(\sum_{i=1}^{2} p_{H_2 i} \cdot F_{H_2 i}\right) + \mathbb{E}\left\{J_S\left(\sum_{j=1}^{4} p_{HC_i} \cdot HC_i(\xi_j) - p_{R_i} \cdot R_i(\xi_j)\right)\right\}$$
$$\forall \xi_j \in \Xi$$
$$\text{s.t.}$$
$$h_F(x_F, u_F) = 0, \qquad g_F(x_F, u_F) \leq 0$$
$$h_S(x_F, u_F, u_S(\xi), x_S(\xi)) = 0, \qquad g_S(x_F, u_F, x_S(\xi), u_S(\xi)) \leq 0 \tag{5}$$

Here the process model and constraints are the same as in the deterministic case (i.e.: *h(·)* and *g(·)*), but evaluated for every scenario, which largely increases the number of variables and equations. The first stage cost corresponds to the production cost of fresh hydrogen, while the second stage includes the expected value of the hydrocarbons processed and the cost of the hydrogen recycles. The aim is to maximize the hydrocarbon load (*HC)* to consumer plants, minimize the use of fresh hydrogen generated in the steam reforming plants (F_H) and minimize the internal recycles of hydrogen (*R*) in the consumer plants, considering all possible values of the uncertainty. u_S refers to the remaining variables of the model.

This TSS formulation is known as deterministic equivalent problem (DEP) since it is solved as a single monolithic optimization problem over all the scenarios.

4.2 Evaluation of the value of the stochastic solution

4.2.1 Scenarios assessed

In particular, a formulation with nine scenarios is presented as case-study in this paper. Table 1 displays details on scenarios conditions, which represent feasible transitions towards a higher hydrogen demand resulting from higher sulphur content crude oil. It is assumed that other realizations are negligible. Therefore, these nine scenarios represent all meaningful ξ_i, such that the probability of occurrence (ρ) of the sum of all equals one (6) All values are presented in per one units (e.g.: 1.1 implies ten percent increase).

$$\sum_{i=1}^{9} \rho(\xi_i) = 1, \qquad a.s. \tag{6}$$

Table 1 – Scenario specific hydrogen demand ($H_{2DEM}(S_i)$), light ends generation ($LIG_{GEN}(S_i)$) and probability of occurrence (Prob(S_i)), for each scenario (S_i). $H_{2DEM}(S_i)$, $LIG_{GEN}(S_i)$ and Prob(S_i) values are presented in per one fractions.

	S1	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**
H_{2DEM}	1	1.1	1.2	1	1.1	1.2	1	1.1	1.2
LIG_{GEN}	1	1	1	1.1	1.1	1.1	1.2	1.2	1.2
ρ	0.36	0.15	0.09	0.15	0.0625	0.0375	0.09	0.0375	0.0225

4.2.2 Typical stochastic formulations

The two-stage stochastic programming problem where the first and second stage variables are considered together resulting in the deterministic equivalent (5), can be interpreted as the recourse problem (RP). In the RP the first stage variables are decided taking into account all possible scenarios, which enlarges the problem as much as scenarios are evaluated. A simplified approach is to consider each scenario separately, assuming the information on the each will be certain once the decision is to be made. Therefore, "perfect information" is assumed for each scenario and computing them separately and weighting the cost function by the corresponding $\rho(\xi_i)$ represents the best theoretical outcome in the long run (PI, a.k.a: wait-and-see). Finally, a second simplification neglects the randomness of the uncertainty and assumes it equal to its weighted average. As a consequence, the realizations of the second stage variables are fixed and the optimization problem becomes a regular deterministic problem, which determines the first stage variables. However, in reality the second stage will reveal all the scenarios in the long run, and at that point one will have to cope with the actual hydrogen demand and previously set hydrogen production. This solution is named the expectation of the expected value problem (EEVP), and is a usual simplification of the TSS problem. These approaches are discussed in detail by Birge and Louveaux (2010).

It is usually interesting to assess whether the two-stage programming stochastic offers an advantage over the two simplified approaches. For this purpose, Birge and Louveaux (2010) proposed the so called value of the stochastic solution (VSS) that is used in this study, as well as the expected value of perfect information (EVPI). The former quantifies the gain in the objective function resulting from considering the randomness of the uncertainty (i.e.: RP), versus its weighted average (i.e.: EEVP). The formula is presented in (7). The latter compares the RP against a theoretical case where demand is certain and known beforehand (i.e.: PI), although this is not realistic.

$$VSS = RP - EEVP \tag{7}$$

$$EVPI = PI - RP \tag{8}$$

4.2.3 Case-study results

Considering actual plant data from a DR solution (discussed in section 2.2), the TSS solutions for the RP, EEVP and PI problem are shown in Table 2. The problem RP involved 15958 variables and 14925 constraints, and required 76.38 CPUs (Intel® Core™ i7 2.50 GHz and 16.0 GB of RAM). In terms of computational efficiency the results are suitable for the online application. Moreover, typical techniques of decomposition (see for reference: Li, Chen, Barton, 2012 and You, Grossmann, 2013) were dismissed as alternative formulations due to the satisfactory results of the monolithic RP formulation. In addition, the EVPI and VSS are presented in the same table to analyze the value of considering uncertainty explicitly. Due to confidentiality reasons, representative but fictitious prices of hydrogen costs and *HC* loads are used in this study.

Table 2 – Results of the implementation of the TSS formulation over the typical stochastic assumptions, i.e.: perfect information (PI), recourse problem (RP), expectation of the expected value problem (EEVP). These are used to calculate EVPI and VSS as suggested by Birge and Louveaux (2010).

PI	RP	EEVP	EVPI		VSS	
k€/h	k€/h	k€/h	k€/h	%	k€/h	%
737.176	735.936	725.014	1.240	0.17	10.923	1.51

It is interesting to notice that with an EVPI of less than one percent it does not seem to be worth investing in additional information from hydrogen demand or light ends generation of the network. It should be born in mind that more information, it almost surely requires equipment investment to undertake better analysis at the refinery laboratory or allocate more resources to the hydrocarbon cuts' properties predictions. However, the VSS shows an improvement of circa one order of magnitude compared to the EVPI, which is due to the incorporation of the stochastic uncertainty in the whole decision-making process from the beginning. In other words, if the uncertainty is estimated when deciding how much hydrogen should be produced and then corrected once the uncertainty reveals (i.e.: EEVP), the objective function is around ten k€ per hour worse than considering the uncertainty from the first stage (i.e.: RP). That is the "price" of simplifying the uncertainty when deciding on the hydrogen production, and neglecting the stochastic nature of hydrogen demand and LIG generation.

The same analysis applies when HC loads of EEVP and RP solutions are compared. For example, if the major hydrogen consumer is analyzed (i.e.: HD3) it could be seen how in most of the scenarios the RP outperforms EEVP (Fig 11). The most favorable results for EEVP are at scenarios S1, S4 and S7, where HD3 maximum load capacity is reached. The rest of the scenarios require HC load to be below HD3 maximum to cope with hydrogen demands. However, RP is capable of meeting hydrogen demand at all scenarios without sacrifice of HC load. This translates directly to the objective function, where HC loads weight around 1000 times more than hydrogen production in volume (5). In addition, RP solution improves CBP purity at all scenarios, which translates into more effective usage of recycled gases across the network contributing to economy of the process network.

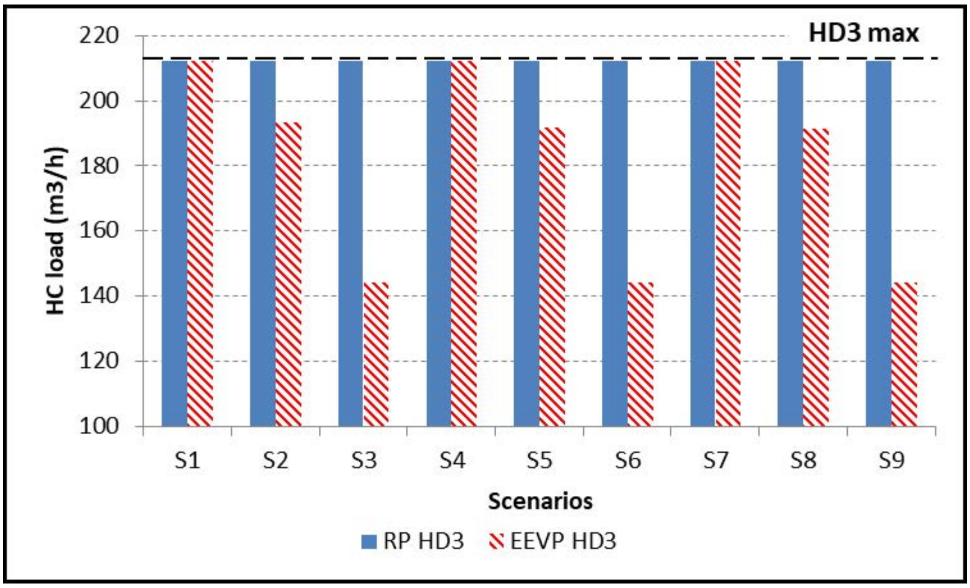

Fig 11 - RP and EEVP solutions for HC loads of process unit HD3.

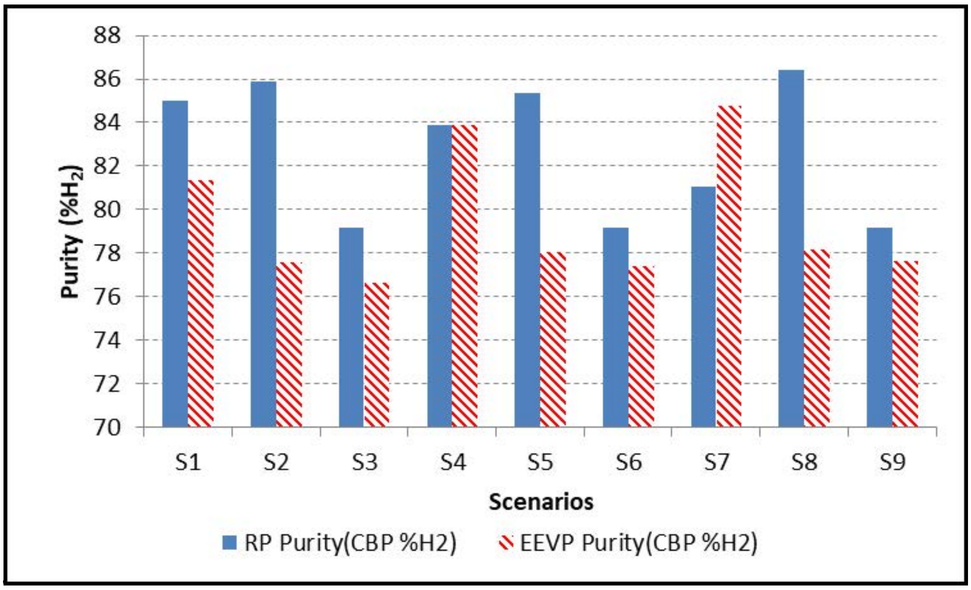

Fig 12 – Low purity header hydrogen purity at scenarios S1 to S9 applying RP and EEVP.

4.3 Considering risk in the decision making process

The previous approach holds when the decisions do not take into account the risk associated to the objective function. Therefore, in the long run the expected valued is maximized regardless of the shape of the probability distribution of the objective function. This sub-section analyzes the formulation and results of applying a TSS approach with a risk measure as objective function.

4.3.1 Conditional Value-at-Risk

First of all, it is important to present the definition of value-at-risk (VaR) as in (9). This risk measurement simply defines a value ω which is the least value of the random variable Ξ, where the likelihood is less than a confidence level 1-α. Another popular risk measure is the conditional value-at-risk (CVaR) defined as in (10), which is actually more useful in optimization for its convexity and other properties such as subadditivity (Pflug, 2000). Equation 11 shows how CVaR and VaR relate to each other, being trivial to see that CVaR is greater than VaR. More details on the characteristics of VaR and CVaR can be found in Rockafellar and Uryasev (2000) and Pflug (2000).

$$VaR_{1-\alpha}(J(\Xi)) \stackrel{\text{def}}{=} \inf_{\omega \in \mathbb{R}} \{\omega | P(J(\Xi) \leq \omega) \geq 1-\alpha\} \tag{9}$$

$$CVaR_{1-\alpha}(J(\Xi)) \stackrel{\text{def}}{=} \inf_{\omega \in \mathbb{R}} \left\{\omega + \frac{1}{\alpha}\mathbb{E}[J(\Xi) - \omega]_+\right\} \tag{10}$$

$$CVaR_{1-\alpha}(J(\Xi)) = VaR_{1-\alpha}(J(\Xi)) + \alpha^{-1}\mathbb{E}[J(\Xi) - VaR_{1-\alpha}(J(\Xi))]_+ \tag{11}$$

$$\begin{aligned} \min_{u_F, u_S(\cdot)} CVaR_{1-\alpha}[J(u_F, u_S(\Xi), x(\Xi))] \Leftrightarrow \min_{u_F, u_S(\cdot), \omega} \; & \mathbb{E}[\omega + \alpha^{-1}\varphi(\Xi)] \\ \text{s.t. } & J(u_F, u_S(\xi), x(\xi)) - \omega \leq \varphi(\xi), a.s. \\ & \varphi(\xi) \geq 0, a.s. \\ & \xi \in \Xi \end{aligned} \tag{12}$$

A practical formulation of the CVaR objective function is presented in (12), the full deduction is illustrated by Artzner et al. (1999). Table 3 shows the results for CVaR and VaR considering the same scenarios presented for RP at three confidence levels 1-α (99% and 95%). Notice that in this case the hydrogen problem is formulated as a minimization problem instead of a maximization as in the previous examples. This is only for practicality of formulation for the CVaR, and does not affect the reasoning behind the analysis.

Table 3 – Results of CVaR, VaR and hydrogen plant H4 at confidence levels 95 and 99%.
[1]Percentage over total production capacity. [2] Intel® Core™ i7 2.50 GHz and 16.0 GB of RAM.

Confidence (1-α)	**$CVaR_{1-\alpha}$**	**$VaR_{1-\alpha}$**	**H4**		**Time**
%	k€/h	k€/h	Nm^3/h	%[1]	CPUs[2]
95	735.88	735.88	37884.06	86.10	71.46
99	735.88	735.88	37884.06	86.15	43.74

According to Table 3 it could be deemed that changing risk from a confidence of 95 to 99 changes very little the detriment in profit for the process, CVaR and VaR in all cases. Moreover, the effect of α is negligible as well in the hydrogen production at H4, see Table 3. In other words, decreasing by five percent the risk of the network profit will be almost indistinguishable in terms of extra hydrogen production. It must be born in mind that *HC* load to hydrogen consumer is at its maximum in all scenarios and confidence levels considered, therefore improvement of profit in scenarios should come from better hydrogen distribution and fresh hydrogen saving from H4. Certainly, this solution is case specific and greatly depends on the actual hydrogen demand circumstances.

An interesting point of view is to compare profit at each scenario for CVaR and risk-free (i.e.: RP) solutions. Fig 13 presents those results. It is important to highlight that considering risk (99 and 95 percent of confidence level) presents a more stable profit across scenarios, at the price of being less on average than the RP. In particular, scenarios six and nine are the ones that RP profit is less than CVaR profits. In the rest, RP profit is greater than CVaR profit. It must be born in mind that these figures are illustrative for the analysis, and not real in terms of profit amounts. Furthermore, the difference between profits is still very narrow and long term results should be analyzed for more robust discussion.

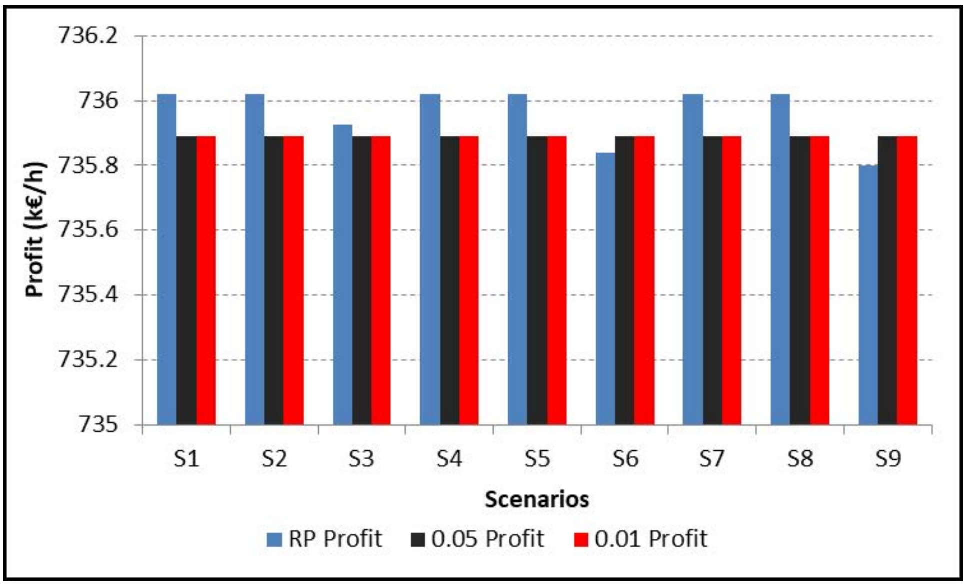

Fig 13 – Profit results over scenarios for RP (without risk distinction), $CVaR_{0.05}$ and $CVaR_{0.01}$.

In overall, the minimization of the weighted average cost of all scenarios considered in the RP does not stop the results obtained in a particular scenario to differ significantly from the optimized average, as the formulation does not include any constraint on the spread or variance of that cost function. To avoid this situation, a measure of the risk of obtaining a cost function significantly worse than the average can be use as cost function instead. However, this so called risk-averse solution comes at the price of lower expected profit in the long run, as it was mentioned before (see Fig 13).

5 CONCLUSIONS

This paper presents the optimization and control system of a hydrogen network in an oil refinery of the Repsol group. It combines data reconciliation and RTO with the implementation of the optimal policies in a commercial DMC+ control system. The optimal policies appear as a set of targets to maximize or minimize within constraints in the LP layer of the DMC+ and are extracted from the analysis of the process and the optimization results proposed by the RTO. This way of implementing RTO has proven to be very effective and allows dealing with dynamics and disturbances as it is executed in real-time with the sampling time of the DMC predictive controller. In addition, the familiarity of the personnel with the DMC interface facilitates the adoption and use of the system and, being based on the DMC models, avoids the possible incoherencies with the ones of the RTO.

In addition this paper studies the advantages of incorporating uncertainty explicitly in the decision making process as a way to deal with the unknown and variable hydrogen demands created by the processing of different crudes. For this purpose, several scenarios were defined and Two-stage stochastic optimization was applied to the problem of optimal hydrogen distribution. On order to evaluate the improvement, two indexes were considered, the Expected Value of Perfect Information, EVPI, and the Value of Stochastic Solution, VSS. The former suggests that little gain is obtained by improving the knowledge on the quality (hydrogen demands) of the hydrocarbon loads being processed, but the VSS indicates that it may be worth to use the Two-stage stochastic optimization in the RTO. Although the results presented are for a particular two-hour period of time, similar conclusions are obtained when studying larger time periods. Finally, the use of an alternative objective function, risk of having a value of the cost function far from what expected, instead of the expected value over all scenarios was considered. More specifically, the Conditional Value at Risk, CVaR, was used. The results show a decrease in the cost function as expected. If the risk factor compensates this is something that should require a deeper analysis with the refinery personnel.

6 ACKNOWLEDGEMENTS

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