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Real-time reconciled simulation as decision support tool for process operation

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ABSTRACT

Decision support tools in the process industry have been gaining relevance, especially for operation under uncertain conditions. This study describes real-time reconciled simulation (RTRS), and analyzes its usefulness as decision-making tool for process operators, especially under unexpected process changes. The proposed methodology is implemented in two case studies in the context of an oil refinery hydrogen network, where both plant and network levels are considered. A what-if analysis is conducted on two case studies, assessing two feasible mitigation actions for each case baseline condition. The focus of the discussion is, nevertheless, on the methodology itself and its general features as decision support tool. The relative error of RTRS for estimation of states and parameters, considering unmeasured disturbances, is satisfactory aligned with industrial standards for online measurements. In terms of mitigation actions, these are assessed with regards to its economic impact on the system in question. It is shown how actions at plant level may be disadvantageous when facing hydrogen demand changes, compared to network-wide mitigation actions. At plant level, it is pointed out the importance of purification units, prevailing over hydrogen make-up for mitigation of demand change. It is highlighted the fact that RTRS complements in a straightforward manner other control operation tools such as model predictive controllers (MPC) and real-time optimizers (RTO). Therefore, it may add to any decision support framework an open-loop component with parameter estimation and forecasting capabilities. Moreover, its potential for training and integration within other tools packages is discussed. Future directions of research are commented such as fully integrated decision support frameworks, including RTRS, MPC and RTO. Additionally, how RTRS may relate to digital twins, including an example of a suitable architecture is introduced, and RTRS role in enterprise-wide decision-making solutions is commented.

1. Introduction

It is well known that process plants are subjected to increasing pressures generated by globalization, increasing competition, environmental regulations, etc. that call for improving energy efficiency, product quality, operation cost, respect to the environment and waste generation, and so on.

In order to fulfill these aims, companies, besides introducing new processes and revamps, are forced to enhance the way they operate their assets and the way they make decisions about production at different levels. As a result, many new technologies had or are being introduced which form what is known as the "automation pyramid" represented in Fig. 1.

From the point of view of operation, Manufacturing Execution Systems (MES), Supervision and Advanced Control, and Basic Control layers play a key role. MES are made up of a set of applications of different nature oriented to production operations management, maintenance, process statistics, quality control and key performance indicators (KPI) management, etc. In batch plants, operation scheduling is in the core of MES, while in continuous ones Real Time Optimization (RTO) applications occupy this place. RTO systems have the function of deciding or recommending the values of the most significant process variables of the production units so that a certain economic cost function is minimized while process and operation constraints are satisfied. This is done

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Abbreviations

AC&O	Advanced control and optimization
BL	Baseline
CM	Condition monitoring
CRO	Control room operator
CV	Controlled variable
DAE	Differential–algebraic equations system
DCN	Distributed control node
DCS	Distributed control system
dll	Dynamic-link library
DM	Dynamic model
DR	Data reconciliation
DS	Dynamic process system
DST	Decision support tool
DSF	Decision support framework
EC	European Commission
ERP	Enterprise resource planning
EOO	Equation and obejct oriented
FG	Fuel gas
FGH	Fuel gas header
FPE	First-principle equations
FPM	First principle models
HAZOP	Hazardous operations studies
HC	Hydrocarbon
HDS	Hydrodesulfurization
HDSLib	Hydrogen dynamic simulation library
HPH	High purity header
HPS	High pressure separator
HS	Hydrogen source
In	Online measurements
ISOPE	Integrated system optimization and parameter estimation
IVP	Initial value problem
KPI	Key performance indicators
LHS	Reactor load heating subsystem
LPH	Low purity header
LPS	Low pressure separator
MES	Manufacturing execution systems
MHE	Moving horizon estimation
MPC	Model predictive control
MU	Make-up
MV	Manipulated variable
NLP	Nonlinear programming
PHD	Process historian server
PROOSIS	Propulsion object-oriented simulation software
PSE	Process systems engineering
PV	Process value
REI	Resource efficiency indicator
RTO	Real-time optimization
RTRS	Real-time reconciled simulation
SP	Set point
WiA	What-if analysis

solving periodically an optimization problem (NLP) of the type:

$$\begin{aligned}&\min_u \quad J(x,u)\\&h(x,u)=0\\&g(x,u)\leq 0\end{aligned} \tag{1}$$

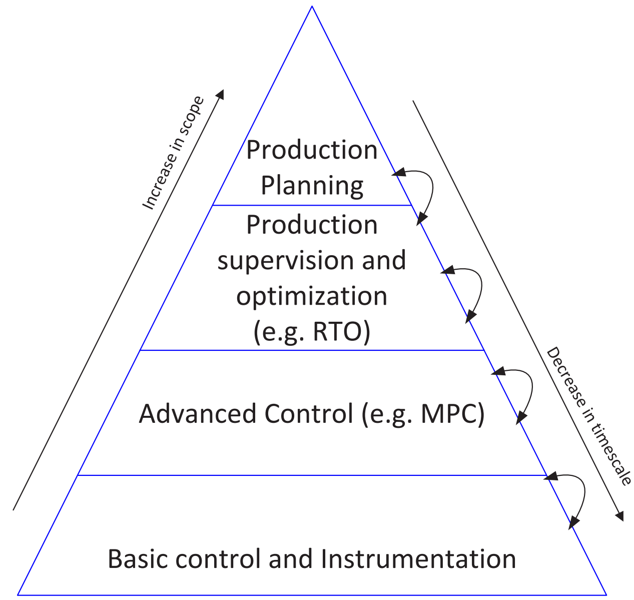

Fig. 1. Automation pyramid. RTO: real-time optimization. MPC: model predictive control.

Where J represents the cost function to be minimized, u are decision variables that corresponds to the degrees of freedom of the process, x are process variables, h is a suitable process model and g are process constraints. The model normally is formulated in steady state and is updated regularly using process measurements. Normally, recognizing that plant measurements may be distorted by noise or biases, a data reconciliation module is added as a way of estimating better values of plant variables and model parameters. In many cases, since the RTO problem is formulated in steady state, a steady-state detector is added to the scheme, as well as a data treatment module to take care of gross-errors or outliers [1], as depicted in Fig. 2.

This generates targets for the next level, providing the best feasible steady state where the plant should operate in order to optimize the cost function $J(u,x)$. These targets are often implemented as set points of Model Predictive Controllers (MPC). As it is well known, MPC utilizes a dynamic model to predict future controlled variables behavior as a function of moves of the manipulated ones, and chooses the best actions that minimize an error function of the predictions with respect to the targets. These actions computed at regular times by the MPC layer are normally implemented in the field by means of single control loops (e.g.: flow, level and temperature) of a Distributed Control System (DCS) installed in the control room, used by operators and technical personnel to deal directly with the process.

In practice, this scheme is implemented in different ways according to the particularities of the plant considered, but it provides a good framework to discuss current challenges faced by the operation of large process plants. The above mentioned tools have provided clear operational advantages and helped to maintain the stability of the plants and improve its performance. There are many successful examples of industrial implementations of these technologies. However, the fact that RTO models are based on steady-state behavior, limits its actual use in complex process plants where steady-state conditions may rarely be reached for long periods of time, which presents another difficulty for actual implementation of RTOs in industry. In general, this may be worked around by changing the scope of the RTO in such a way that time at steady-state conditions is more likely in the long run, however this may leave out of scope some key process

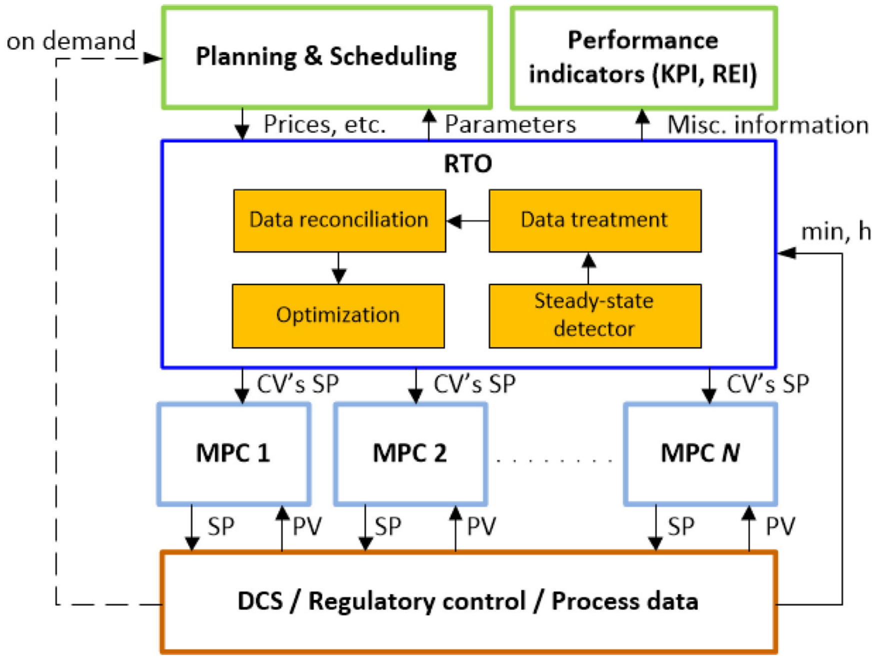

Fig. 2. Information flow around RTO tools, including the typical architecture of an RTO and its information exchange with Planning and Scheduling (upper hierarchical level) and *N* MPC modules (lower hierarchical level), and process data updates. CV: controlled variables. SP: set-points. DCS: distributed control system. PV: process values. KPI: key performance indicator. REI: resource efficiency indicator.

variables which is certainly disadvantageous to say the least. Hence, defining the scope of the RTO is critical for succeeding and requires significant knowledge of the process (or support from those who are subject matter experts of units related to the RTO) and good judgment to understand the trade-offs of larger scopes vs smaller scopes. Additionally, it is important to keep in mind that, first, quite often they operate more or less independently using different models not always coherent, which sometimes generates problems and reduces the benefits it could bring and, second, they deal with only some, but not all, the decisions that daily operation requires.

The first point refers not only to the use of different models in the RTO and MPC layers, quite often static, nonlinear and based on first principles in RTO, and dynamic, linear and data based in MPC, but also to the different time scales they operate, hours in RTO, minutes in MPC. Often, different company departments are responsible for their operation and maintenance, which leads to additional incoherence between models. This calls for an effective integration of levels, in particular between RTO and MPC [2,3]. Several proposals have been made in the literature, of which economic MPC (EMPC) is perhaps the best known [4–6]. EMPC uses directly an economic target in the controller instead of a quadratic error function with respect to set points and may incorporate a dynamic nonlinear process model, solving many of the above mentioned integration problems. Nevertheless, its use in large scale processes is not realistic, due to the size and complexity of the resulting dynamic optimization problem that must be solved on-line in a safe and consistent way. Integration of RTO and enterprise resource planning (ERP) tools is also an important topic but out of the focus of this paper.

Regarding decision making, the second point, is as important as the integration of RTO and MPC [7,8]. Operators and technical personnel face many operational decisions regularly using their experience and knowledge of the process. These may be motivated by aspects not considered normally in RTO concerning, for instance, people, safety, availability of equipment, state of catalysts, and so on, or respond to transient changes in the plant that require human intervention. However, when it comes to large scale processes, its complexity sometimes prevents front-line personnel from adequately predicting the consequences of these operational decisions on production. Simulation techniques have been proposed since long ago as a way of offering some help in dealing with these problems creating an environment that facilitate the evaluation of the solutions proposed by different tools or people regarding plant conditions, though its use has not spread very much. Partly, this may be due to the fact that simulation is often used in isolation from other tools, with static models and off-line, while decision makers in the control rooms require dynamic real-time tools able to forecast the process behavior as a function of the current state of the process and intended decisions. Nevertheless, nowadays, as a result of the adoption of digitalization in the process industries and advances in the simulation environments, new conditions have been created so that dynamic simulation, combined with other tools, can form efficient decision support systems.

This paper deals with the above mentioned problems of tools integration and decision making as a support for process operators based on novel simulation framework. It proposes an architecture that efficiently combines dynamic simulation, RTO and MPC as an effective decision and operation support system in continuous process plants. The paper describes such a framework with reference to a large scale industrial process: the hydrogen network of an oil refinery located in Spain, involving 18 plants linked by a complex distribution network. Moreover, it discusses its implementation, operational requirements and lessons learnt, with special reference to the simulation framework developed.

The paper is organized as follows. After the introduction, a brief overview of the main aspects of crude oil refinery hydrogen networks and the specific configuration of the case study addressed is given in Section 2. Then, the architecture of the decision support system is presented and discussed in Section 3, as well as the integration of modules. Next, Section 4 is focused on what we call real-time reconciled simulation framework. Finally, in Section 5, the paper presents some case studies with their respective results and discussion. Conclusions are given in Section 5, including future work directions.

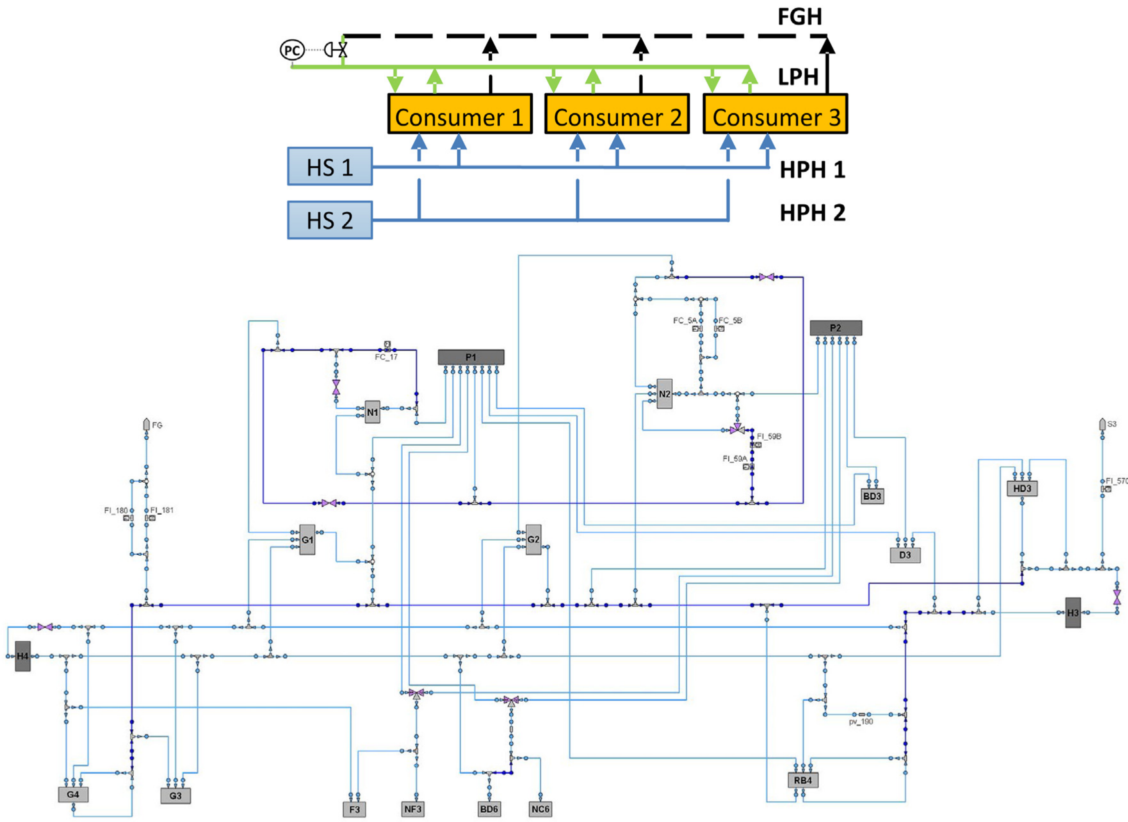

Fig. 3. Top: generic H_2 network diagram with sources (HS1/2), consumers 1–3, high purity headers (HPH 1/2), low purity header (LPH), and fuel gas header (FGH). Bottom: Petronor, refinery H_2 network in Muskiz, Spain [9]. Gray boxes represent process plants.

2. Hydrogen networks in crude oil refineries

Hydrogen (H_2) is used in oil refineries mainly for removing sulfur from hydrocarbons in order to comply with environmental regulations (known as hydrodesulfurization process). In addition, hydrogen is consumed in hydrocracking units for converting long chain hydrocarbons (a.k.a. "heavy"), received from vacuum distillation unit bottoms, into shorter chain molecules (a.k.a. "light"), which are more valuable fuel blending components. Hence, H_2 has become a key utility in the operation of the refineries. Currently, high purity hydrogen is provided either by an external supplier and delivered by pipeline to the refinery network or produced internally from steam reforming plants. Other hydrogen sources are platforming units, aimed at increasing the octane number of gasolines, which produce low purity hydrogen as a by-product fed to the hydrogen network. Whichever the source is, hydrogen is finally distributed to individual consumer plants through a set of headers and pipelines, in a complex network arrangement. For instance, Petronor refinery hydrogen network comprises 14 consumer plants, two steam reformers and two platformers, is presented in Fig. 3 (bottom). Moreover, headers are usually sorted by H_2 purity, namely: high (HPH), low (LPH) or fuel-gas (FGH). HPH contain H_2 purities over 90% and are fed by steam reformers. LPH contain over 70% H_2 purity and are fed by platformers and recycle purge from consumers, see Fig. 3 (top). Typically, excess gases from LPH and consumers, as well as other non-recyclable off-gases (e.g.: less than 70% H_2 purity), are collected by a fuel gas header (FGH) and used as fuel for burners across the refinery. Thus, only HPH and LPH gases are used as make-up (MU) gas to the consumer units.

A simplified schematic of a typical HDS plant can be seen in Fig. 4. The high sulfur hydrocarbon (HC) feed is mixed with treatment gas (typically around 85%–90% hydrogen content, and high pressure) coming from different sources (high and low purity headers, HPH and LPH respectively). This cold mixed stream is heated to reaction temperature, around 300–400 °C, by heat exchangers and a furnace (reactor load heating subsystem, LHS) before going into the reactor. This untreated hot stream reacts in the catalyst fixed bed of the reactor, where the actual desulfurization and other side reactions take place. Due to the exothermal nature of the reactions, the outlet stream is used to preheat the cold stream load in the heat exchangers within the LHS. The next stage of the process is the separation of gas and liquid, for this purpose the high pressure separator (HPS) is fed with the cooled reactor outlet, and produces two outlets: High pressure sour gas (rich in hydrogen sulfide, H_2S) and medium or low pressure mixed gas and HC.

Another key point related to the operation of the reactors is purity management. As mentioned before, the gas recycled from the separation units (HPS) has lower purity than the treatment gas fed to the reactor, but its purity can be increased using permeation membranes or, after being sent to LPH, reused in other plants either directly or mixed with fresh hydrogen to increase its purity.

Hydrogen cannot be stored efficiently, and an excess of hydrogen has to be kept in the reactors to avoid catalyst deactivation. As a result of this, 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 should be distributed 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 the most important economic target: the maximization of the hydrocarbon loads processed in the hydrodesulfurization plants, which may be limited

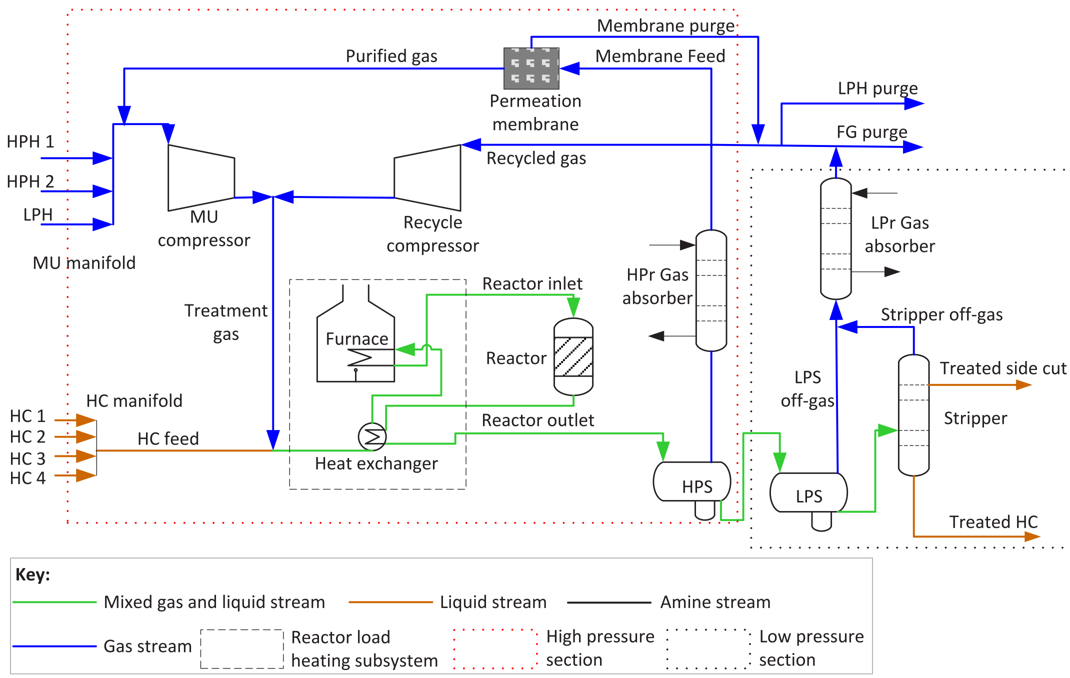

Fig. 4. Simplified schematic of a generic hydrodesulfurization (HDS) plant. HPH: High purity gas header. LPH: Low purity gas header. HC: Liquid hydrocarbon; MU: Make-up. FG: Fuel gas. HPS: high pressure gas/HC separator. LPS: Low pressure gas/HC separator. HPr: high pressure. LPr: low pressure.

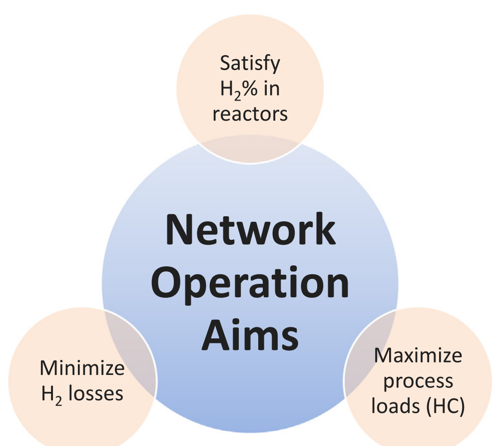

Fig. 5. Hydrogen network operation aims: satisfying minimum H_2 purity in reactors, maximizing HC processed (consistently with plant scheduling), and minimizing pure H_2 losses to FGH.

by the hydrogen available and the production aims established 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. Certainly, decisions must satisfy all process constrains imposed by the equipment, operation, safety, targets or quality.

In summary, hydrogen network operation aims should consider three dimensions, i.e.: H_2 purity in reactors, H_2 losses to FGH and HC processed in consumer plants. Due to the impact of each dimension in the process economy, an optimal operation should consider the following broad directions (see Fig. 5 for a summary of operating aims at a glance): H_2 purity in reactors and H_2 losses, should be as low as possible, while HC processed should be maximized.

3. Decision support framework

As mentioned above, optimal operation of the network, or any other complex process, requires proper tools at different levels, including support for non-automated decisions. Our vision of the architecture of a system oriented to fulfill these aims, more than the rigid hierarchical structure of Fig. 2, comprises a set of functional modules organized in a decision support framework, as portrayed in Fig. 6. This would provide integral visibility across operations within a process network to aid decision makers.

Besides the production plants, DCS and Historian, Fig. 6 shows three groups of functional blocks: those related to the operation of a RTO system appear in orange, those related to MPC in yellow while two new blocks in green are related to real-time simulation. In relation to the traditional architecture of Fig. 2, three main changes can be observed: The first one is an architecture that moves towards what could be considered a mesh more than a hierarchy. This point is related with recent trends and standards for the new generation of control systems like the proposal of the Open Process Automation Forum (OPAF): the O-PAS^{TM} (Open Process Automation Standards) which promotes a modular architecture characterized by open standard interfaces between elements [10]. The automation pyramid is eliminated and replaced by a flat structure where each system can communicate with each other through distributed control nodes (DCN) across a connectivity framework as portrayed in Fig. 7.

The apparently unconnected RTO and MPC modules, along with the real-time reconciled simulation (RTRS) module, in a scheme oriented to operate in real-time is addressed in the subsequent Sections 3.1 and 3.2.

3.1. Integrating RTO solutions into MPC

As mentioned in the introduction, the classical cascade implementation of RTO–MPC in which RTO executes at slow pace a static, nonlinear optimization and fixes the set points of a linear MPC executed at higher frequency, though conceptually clear and easy to perform, presents several issues. Among them, it can be

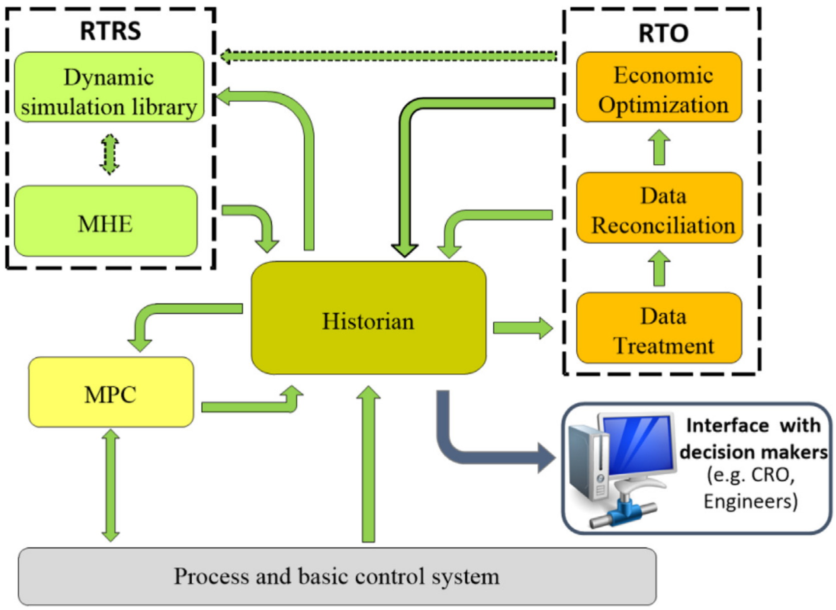

Fig. 6. Block diagram of the proposed decision support framework showing the information flows. LP: linear programming. CRO: Control room operator. DMC: dynamic matrix control. MHE: moving horizon estimation. RTRS: real-time reconciled simulation.. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

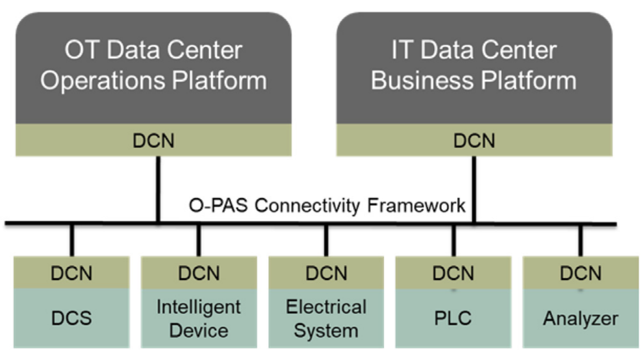

Fig. 7. O-PAS modular architecture. DCN standard enables communication of non-O-PAS compliant modules through the connectivity framework. Modules can exchange data and information across the system in a straightforward manner. *Source:* [10].

highlighted the fact that RTO solutions corresponds to an ideal optimal steady state of the processes but, in practice, process plants are rarely in a steady state. Connected to this, the slow execution period of RTO implies that adaptation to any new condition only takes place from time to time, without early reaction against significant disturbances, which limits the benefits of RTO.

3.1.1. Data reconciliation and RTO

This is the case in the hydrogen network taken as reference where a RTO system is in operation involving the 18 plants described in Section 2. The system collects 171 flows and 18 purity measurements, plus other variables and configuration parameters (temperatures, pressures, valve openings, etc.) totaling around 1000 variables, averaging them in two-hour periods to smooth the effects of transients and disturbances. Notice that, in spite of this number, there are many more variables that are not measured and many of them are not reliable. After analyzing and filtering them, they are fed to a data reconciliation module, which plays a central role in the architecture of Fig. 6. This module solves periodically an optimization problem that provides estimations of all plant variables consistent with a process model and constraints and having values as close as possible to the process measurements. The model involves more than 4400 variables and 4700 equality and inequality constraints with flows, purities, molecular weights of hydrogen and light ends and hydrogen consumption in the reactors as main variables. It is based on stationary mass balances and reduced order models of some special units like separators and membranes. The model is adapted automatically to structural changes, like a plant being shut down. The NLP problem is solved using IPOPT in the GAMS environment in a few minutes.

Then, using the updated model, another optimization problem is solved every two hours in the RTO module, using a cost function that aims to: maximize the hydrocarbon load to consumer plants, minimize the use of fresh hydrogen generated in the steam reforming plants, and minimize the internal recycles of hydrogen in the consumer plants, which is linked to the operation of the recycle compressors. It considers : the reconciled process model, a set of operational constraints, and the refinery planning specifications. Main decision variables include: production of fresh hydrogen, feeds to consumer plants, hydrogen flows and recirculation, purges, purities and membranes operation, involving around 2000 variables and 1800 constraints and is solved also in the GAMS environments in a few minutes. Nevertheless, taking into account what was discussed at the beginning of this Section 3.1, the solutions found are not passed directly as set points to a MPC. Instead, the procedure displayed on Fig. 8 was used.

3.1.2. Implementation of RTO and MPC

The first step in the methodology involves analyzing the solutions provided by RTO and extract common features or policies that correspond to the optimal operation. Examples in the hydrogen network problem can be to minimize the flow from H4 to H3 headers, or reduce the purity in the stream out of the high pressure separators as much as possible. Note that these are not specific values for set points of any variable but directions for the entire network to operate with minimum cost, which can be translated formally in terms of an optimization problem. The second step takes advantage of the two-layer architecture of many industrial MPC controllers like the DMC+ which incorporate

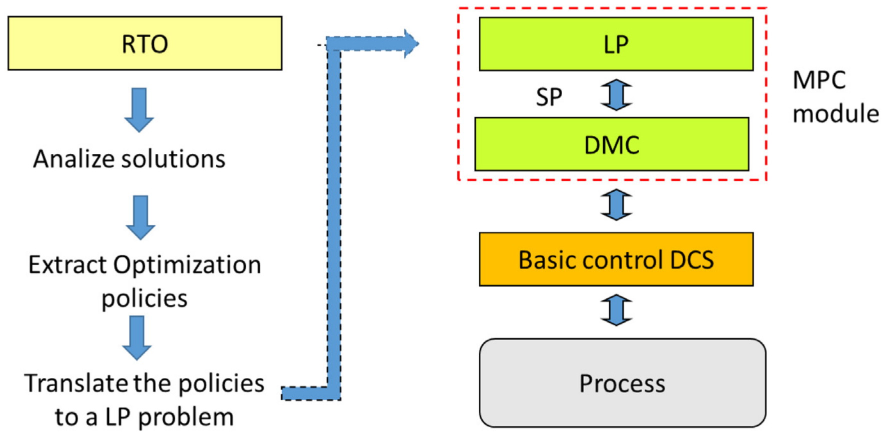

Fig. 8. *Left hand side* - Implementation of the RTO generated policies as targets in the LP layer of the MPC module. *Right hand side* - the local LP optimizer sets of future values of the DMC set points.

internally a linear programming (LP) optimizer that generate targets for a DMC controller [11]. The optimal policies of the RTO can be then implemented as targets in the LP layer which will generate specific set points (SP) to the DMC according to the process conditions. In this way, the MPC operates independently, adapting the policies extracted from the RTO to the process state. In essence, network-wide optimization results are transferred to the MPC by the operators in an open-loop manner or incorporated in the reduced LP function in the MPC if significant discrepancy is observed. A comprehensive discussion of this approach towards RTO–MPC integration is described by [12,13]. This reminds the idea of self-optimizing control of implementing optimization as control introduced by [14]. Nevertheless, the implementation is different because here there are no self-optimizing variables to control but policies to follow. The actual implementation in the refinery was done by the Petronor team and includes a DMC that covers the six most important plants of the network from the point of view of hydrogen management, trying to balance benefits obtained with simplicity of implementation. The controller operates only on key variables such as the set points of hydrocarbon loads to the consumer units, fresh hydrogen production, hydrogen feed to the consumers from the high purity header and supply of hydrogen from one of the platformer plants. It is executed every minute bringing consistent benefits. More detail about the operation of the network can be found in [15] and [12].

Note that, even if the RTO solutions are not implemented in real-time as it is an open-loop framework, both the data reconciliation and the RTO keep running on-line generating both, useful information about the hydrogen network and indications on how to command it optimally that are available through the process information system, remaining a part of the decision support framework.

3.2. Real time reconciled simulation

As mentioned in the introduction, there are many operational decisions that operators and technical personnel have to make due to changes in the plant or operating conditions that require human intervention. In the same way, revising or accepting what is been suggested by the RTO when new situations or constraints realize requires human action and judgment. In large scale and complex processes like the hydrogen network, it is difficult to predict the consequences of some operational decisions on production. Simulation can offer help in this task, allowing the evaluation of the solutions proposed by different tools or people regarding new plant conditions. That is why the module RTRS appears in Fig. 6.

However, in order to be useful and predict the future process evolution as a function of time and the intended decisions, the simulation has to be dynamic and must be properly initialized in real-time at the current process state, not to mention that the model has to be maintained properly updated. In order to perform the initialization and updating in real time, under user demand, the dynamic simulation must be integrated with other modules of the decision support and operation framework, namely the moving horizon estimation (MHE) and the data reconciliation modules. Integration with the RTO is also required in order to allow an easy evaluation of its proposals. The data reconciliation (DR) results can be used to update many model parameters but current state estimation requires past dynamic data obtained through the historian system and integrated estimation tools such as MHE that constitute the remaining block of the decision support framework.

In this context, real-time reconciled simulation (RTRS) is defined as a system simulation, intended to be used in parallel with the process, in which all current parameters and states (measured and unmeasured) arise as a result of a DR based on past and current plant data. Moreover, it is capable of representing the future condition of the system within a simulation time horizon, provided that certain boundaries or manipulated variables (MV) are given within that horizon.

From its definition, RTRS can be seen as a real-time simulation tool which incorporates parameters and states estimations based on current plant data. These capabilities motivate the interest in developing further RTRS applications. In particular, its combination of open-loop decision support and plant forecasting features, are the most outstanding outcomes of these tools. Fig. 9 shows a schematic of a decision support framework with a RTRS application, where, past system states, along with past and current manipulated variables, are captured online and utilized alongside a dynamic model, to estimate the current state of the system and its parameters. However, RTRS are challenged to effectively integrate plant forecast features (based on current plant status), with ease of implementation by end-users, e.g. control room operators, plant engineers, due to the complexity of integrating simulation and optimization tools towards real-time simulation for process operation.

4. Simulation environment

This section describes the models used in the simulation and the simulation environment as well as the initialization procedure.

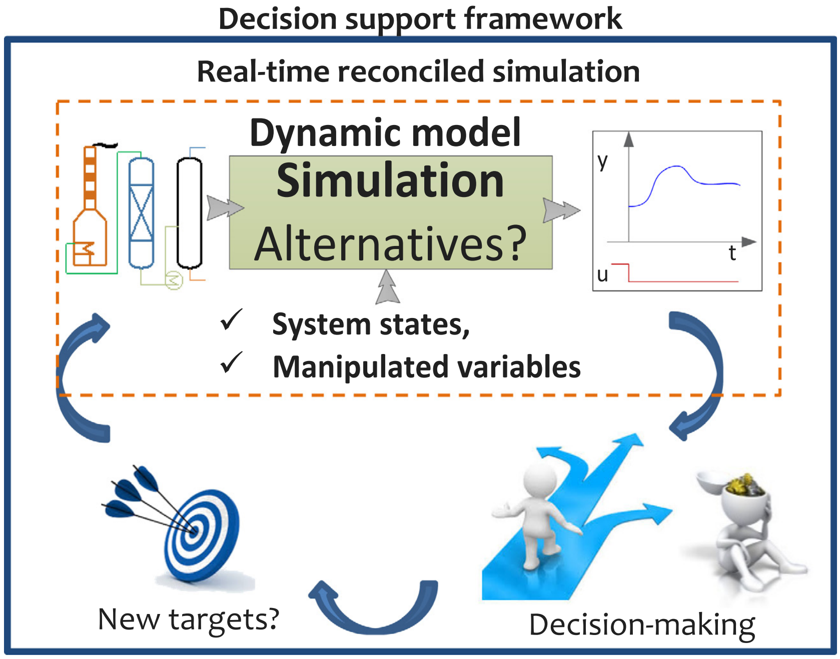

Fig. 9. Decision support framework information flow with a real-time reconciled simulation application.

4.1. Simulation model and framework

The models used in the simulation module are coherent with the ones used in data reconciliation or RTO, so that direct transfer of values is possible, but they incorporate dynamics where appropriate.

All pieces of equipment comprising the plants and their connections, as well as the network connections are formulated as first principles models and as simple as possible trying to balance a good description of the key phenomena in the hydrogen network with the necessary computational performance. The model of the distribution network is based on mass balances of hydrogen (H_2) and light ends (considered altogether as a single pseudo-component, *LIG*). In the models, F stands for gas flows, X are hydrogen purities, and MW refers to molecular weights, while liquid streams are defined by: HC (liquid hydrocarbon flowrate), ρ_{HC} (HC density) and MW_{HC} (HC molecular weight). Each k node has outlets i and inlets j streams (2.a–d). Taking into account the difference in time constants between pipelines and reactors and other equipment, the models of the pipelines are considered static.

Models for reactors (3.a–i), membranes (4.a–e), separation units (5.a–j), compressors and headers (2.a–d) incorporate other first principle and reduced order equations. Their models consider two basic mechanisms of H_2 consumption: chemical reaction (in reactors) and solubility losses (in separators). Simplified first order dynamics are considered in reactors, since H_2 is required in great excess compared to HC to protect catalysts premature deactivation. Reduced order models are used for permeation membranes fitting their parameters to historical plant data following methodologies of previous works by [16] and before by [9]. Table 1 presents a description of all variables and subscripts, while engineering units used in this study are provided in Table 2. In addition, the model incorporates a quantification of process economy (6), which is used for assessing the impact of different operations (a.k.a. set of actions SC) on profits over scenarios. Thereby, the economic impact of changes is transparent to decision makers. In particular, for any given number of scenarios considered, the best alternative is the one that satisfies all operational constraints, at the time it provides the highest process profit (6).

At all nodes N:

$$\sum_{i,\ out} F_{k,i} = \sum_{j,\ in} F_{k,j} \quad \forall\ k\ \in N \tag{2a}$$

$$X_{H2,\quad k} \cdot \sum_{i,\ out} F_{k,i} = \sum_{j,\ in} X_{H2,\quad k,\ j} \cdot F_{k,j} \quad \forall\ k\ \in N \tag{2b}$$

$$MW_k \cdot \sum_{i,\ out} F_{k,i} = \sum_{j,\ in} MW_{\ k,\ j} \cdot F_{k,j} \quad \forall\ k\ \in N \tag{2c}$$

$$100 \cdot MW_k = MW_{H2} \cdot X_{H2,\ k} + (100\ -\ X_{H2,\ k}) \cdot MW_{LIG,\ k} \quad \forall\ k\ \in N \tag{2d}$$

At all reactors r:

$$F_{in,\quad r} = F_{out,\quad r} + RD_{H2,\quad r} - RD_{LIG,\quad r} \tag{3a}$$

$$F_{in,\quad r} \frac{X_{in,\ r,H2}}{100} = F_{out,\quad r} \frac{X_{out,\ r,H2}}{100} + RD_{H2,\quad r} \tag{3b}$$

$$F_{in,\quad r} MW_{in,r} = F_{out,\quad r} MW_{out,r} + RD_{H2,\quad r} MW_{H2} - RD_{LIG,\quad r} MW_{LIG,r} \tag{3c}$$

$$RD_{H2,\quad r} = HC_{in,\quad r} \cdot rd_{H2,\quad r} \tag{3d}$$

$$RD_{LIG,\quad r} = HC_{in,\quad r} \cdot rd_{LIG,\quad r} \tag{3e}$$

$$rd_{H2,\quad r} + \tau_{H2,r} \cdot \frac{d\left(rd_{H2,r}\right)}{dt} = rd_{H2,r,SS} \tag{3f}$$

$$rd_{LIG,\quad r} + \tau_{LIG,r} \cdot \frac{d\left(rd_{LIG,r}\right)}{dt} = rd_{LIG,r,SS} \tag{3g}$$

$$HC_{in,\quad r} = \frac{d\left(HC_{out,\quad r}\right)}{dt} \cdot \tau_{HC,\quad r} + HC_{out,r} \tag{3h}$$

$$W_{HC,in,\quad r} = W_{HC,out,r} - RD_{LIG,\quad r} \frac{MW_{LIG,r}}{LM} \tag{3i}$$

$\forall r \in Reactors$

At all permeation membranes z:

$$F_{in,\quad z} = F_{o,\quad z} + F_{pg,\quad z} \tag{4a}$$

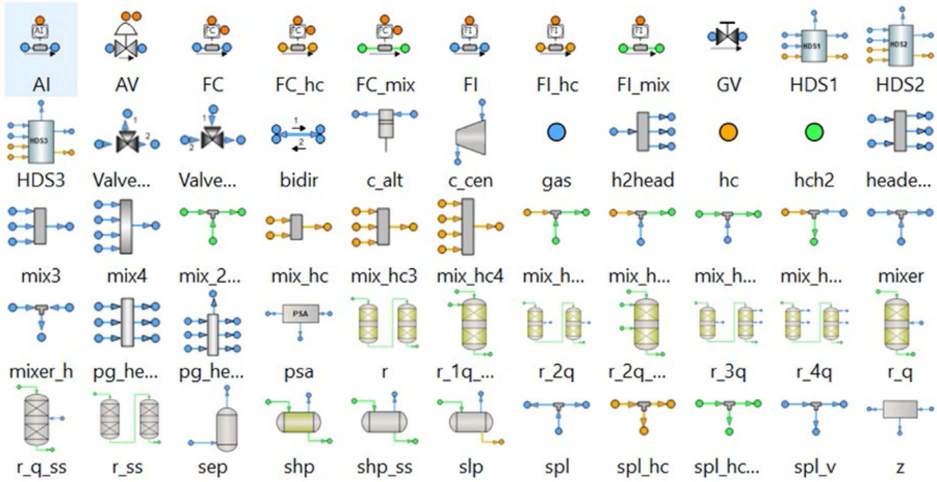

Fig. 10. Components of the dynamic hydrogen network library used to build models by interconnection.

$$F_{in,\ z}\frac{X_{in,\ z,H2}}{100} = F_{o,\ z}\frac{X_{o,\ z,H2}}{100} + F_{pg,\ z}\frac{X_{pg,\ z,H2}}{100} \tag{4b}$$

$$F_{in,\ z}MW_{in,z} = F_{o,\ z}MW_{o,z} + F_{pg,\ z}MW_{pg,z} \tag{4c}$$

$$X_{o,\ z,H2} = a\frac{F_{pg,z}}{F_{in,z}} + b\cdot X_{in,\ z,H2} + c \tag{4d}$$

$$MW_{in,\ z,LIG} = MW_{o,\ z,LIG} \tag{4e}$$

$\forall z \in Permeation\ membranes$

At all separators *se*, (13.h-j) do not apply to low pressure separators:

$$ksol_{se,gasHC} = \frac{22.415\cdot G_{out,se}\left(Y_{out,se,H2}+Y_{out,se,LIG}\right)}{G_{out,se}\cdot Y_{out,se,HC}\left(\frac{MW_{HC}}{\rho_{HC}}\right)} \tag{5a}$$

$$ksol_{se,H2HC} = \frac{22.415\cdot G_{out,se}\cdot Y_{out,se,H2}}{G_{out,se}\cdot Y_{out,se,HC}\left(\frac{MW_{HC}}{\rho_{HC}}\right)} \tag{5b}$$

$$ksol_{se,MWLIG} = \frac{MW_{out,se,LIG}}{MW_{Gout,se,LIG}} \tag{5c}$$

$$ksol_{se,H2gas} = \frac{ksol_{se,H2HC}}{ksol_{se,gasHC}} \tag{5d}$$

$$G_{in,\ se}\left(100-Y_{in,HC}\right) = F_{out,\ se} + G_{out,\ se}\left(100-Y_{out,se,HC}\right) \tag{5e}$$

$$G_{in,\ se}Y_{in,se,H2} = F_{out,\ se}X_{out,se,H2} + G_{out,\ se}Y_{out,se,H2} \tag{5f}$$

$$G_{in,\ se}\left(100-Y_{in,HC}\right)MW_{Gin,se} = F_{out,se}MW_{out,se} + G_{out,\ se}\left(100-Y_{out,se,HC}\right)MW_{Gout,se} \tag{5g}$$

$$HC_{in,\ se} = \frac{d\left(HC_{out,\ se}\right)}{dt}\cdot\tau_{HC,\ se} + HC_{out,se} \tag{5h}$$

$$ksol_{se,gasHC} + \tau_{se,gasHC}\cdot\frac{d\left(ksol_{se,gasHC}\right)}{dt} = ksol_{se,gasHC,SS} \tag{5i}$$

$$ksol_{se,\ H2HC} + \tau_{se,H2HC}\cdot\frac{d\left(ksol_{se,H2HC}\right)}{dt} = ksol_{se,H2HC,SS} \tag{5j}$$

$\forall se \in Separators$

$$Profit_{SC} = \sum_{i=1}^{U} pr_i\cdot HC_{SC,i} - \sum_{i=1}^{H} ct_{HS,i}\cdot HS_{SC,i} - \sum_{i=1}^{RH} ct_{LPH,i}\cdot LPH_{SC,i} \tag{6}$$

The models were coded in the modeling environment EcosimPro®/PROOSIS® [17], an equation and object oriented (EOO) modern simulation software, with straightforward communication capacity with other software packages, such as MS Excel® and C++. In particular, its capability to model reuse and numerical performance is highly appreciated. A graphical model library with the different components that appear in the hydrogen network was developed as a tool for developing models for the whole network. The main symbols associated with the components of the library can be seen in Fig. 10.

Models of the different plants and the hydrogen network were built by interconnecting the appropriate components. After parameterizing them, a partition can be created as a function of the degrees of freedom of the process and finally C++ executable code with all required numerical algorithm is created automatically ready to be run. One example of schematic corresponding to the Petronor hydrogen network can be seen in Fig. 11.

4.2. Moving horizon estimation implementation

As mentioned before, on-line use of the simulation models requires proper initialization of the model. Current value of many model parameters can be incorporated from the last data reconciliation run, but the current value of some states may not coincide with the averaged value provided by this module and stored in the process information system. In this context, a module is required to estimate current time unknown states and parameters, based on online and historical measurements. In this way, the RTRS is able to support on-line plant forecasting, aiding operators in their decision-making process for future actions. These might be intended for actual open-loop control action or to support scenario-based decisions, operators training or other forms of operation assessment. Fig. 12 presents a schematic illustrating of all the previous components of the system in question.

The state estimation stage is addressed applying the so called, and well known, moving horizon estimation (MHE) technique, which has several successful implementation examples as [18–21]. For further theoretical reviews and comprehensive analysis on the MHE method refer to [22,23].

Thereafter, starting with current values of states and parameters as a result of the state estimation, the simulation is computed for forecasting future behavior of the system. The dynamic state estimation problem to be solved in MHE is presented next.

Given:

- a DAE, i.e.: dynamic model (DM),
- plant measurements y and information
- previous manipulated variables' (MVs) values, u

Estimate state variables at time t-N and possible disturbances for the interval [t-N, t] such that the difference between DM variables response and plant data is minimized along the past

Table 1
Descriptions of variables and subscripts.

ct	Cost of gas stream in k€/Nm^3.
F	Gas flow, in Nm^3/h
G	Mixed gas and liquid stream, in kmol/h.
HC	Liquid hydrocarbons flow, in m^3/h.
HS	High purity H_2 source flowrate, in Nm^3/h.
$ksol_{se,gasHC}$	Total gas solubility in hydrocarbons at separator se, in Nm^3/m^{3}HC.
$ksol_{se,H2HC}$	H_2 solubility in hydrocarbons at separator se, in Nm^3/m^{3}HC.
$ksol_{se,MWLIG}$	MW_{LIG} gas/liquid solubility coefficient, dimensionless.
$ksol_{se,H2gas}$	H_2 content in solubilized gas at separator se, in %vol.
LM	Mol-Volume ratio for gases at 0 °C and 1 atm, 22.414 Nm^3/kmol.
LPH	Low purity gas pipeline header flowrate, in Nm^3/h.
MW	Molecular weight, in kg/kmol.
pr	Price of liquid hydrocarbon in k€/m^3.
$Profit$	Profit of the process in k€/h.
rd	Specific demand (rd_{H2}) or generation (rd_{LIG}), in Nm$^3H_2$/m^{3}HC.
RD	Reactor demand (RD_{H2}) or generation (RD_{LIG}), in Nm^3/h.
W	Mass flow, in kg/h.
X	H2 or LIG fraction in a gas stream, in %vol.
Y	Total molar fraction of a gas and liquid stream, in %.
ρ	Density of a liquid stream, in kg/m^3.
τ	Hydraulic time constant, in h.
Subscripts	
in	The variable represents an inlet.
k	A node within the network.
H	Set of high purity H_2 sources across the network.
N	Model node.
o	The purified gas of a permeation membrane.
out	The variable represents an outlet.
pg	The gas purge of a permeation membrane.
lb	Lower bound
r	A reactor within the network.
RH	Set of make-up gas streams from LPH across the network.
se	A separator within the network.
SC	Scenario.
U	Set of process units across the network.
ub	Upper bound
z	A purification membrane within the network.

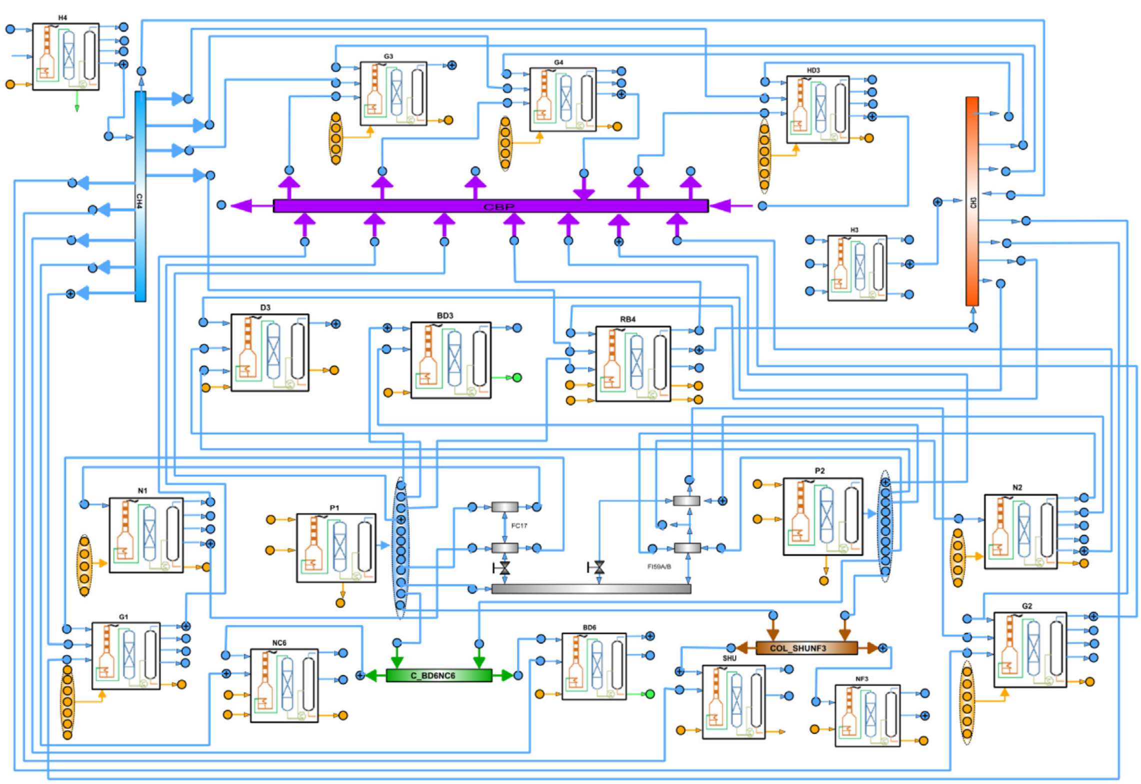

Fig. 11. Schematic of the hydrogen network generated with EcosimPro®/Proosis® [17].

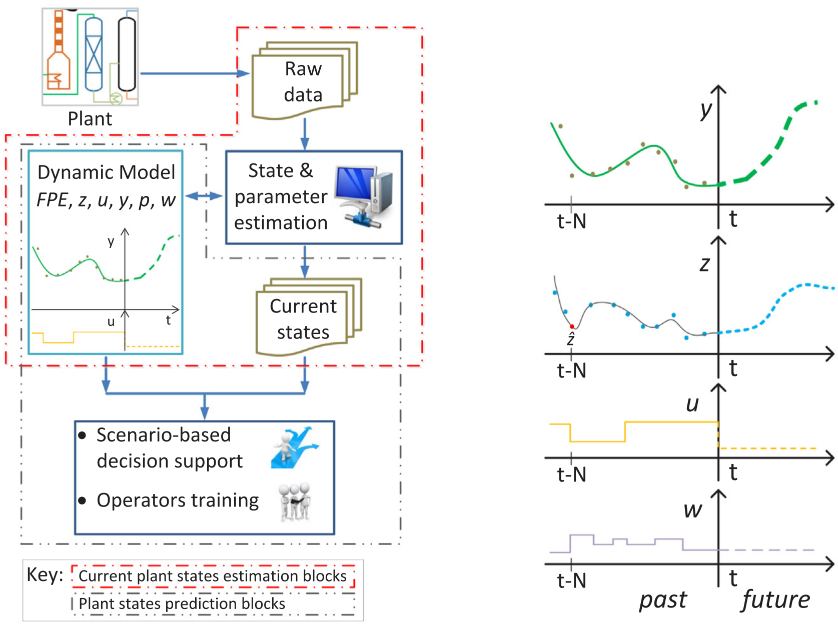

Fig. 12. *Left hand side* - Framework and information flowchart addressed. FPE: first-principle equations. z: states. u: manipulated variables. y: model outputs. p: parameters. w: disturbances. *Right hand side* - A representation of y, z, u and w, on the same timeline. Full lines represent continuous variables in the past, while dashed lines represent those variables in the future. Dots correspond to discrete data or estimations in the past *t-N* instants.

Table 2
Engineering units used, unless explicitly stated otherwise.

Liquid flow	Gas flow	Gas purity	Molecular weight	Time	Cost/Profit
m^3	Nm^3/h	%vol	kg/kmol	h	Euros/h

rolling horizon of N sample times. Once these values are known current states can be calculated by simulation of the DM from *t-N* to *t*.

Eqs. (3)–(11) show the mathematic formulation of the MHE problem, given a continuous-time dynamic system.

$$y_m(t) = h\left(z\left(t\right), u\left(t\right), p\right) \ , \tag{7}$$

$$f\left(z\left(t\right), \dot{z}\left(t\right), u\left(t\right), p, w(t)\right) = 0, \quad z\left(0\right) = z_0, \tag{8}$$

$$I^{(N)}{}_k \triangleq col\left(y_{k-N}, \ldots, y_k, u_{k-N}, \ldots, u_{k-1}\right), \tag{9}$$

$$\Delta w_k = w\left(k\right) - w(k-1), \tag{10}$$

$$k = 1,\ 2,\ \ \ldots,\ \ N \tag{11}$$

Where z represents the state vector, u the control vector and w the unmeasured disturbance of the system, $\dot{z}$ is the derivative of z, and p the vector of parameters (7). Model output y, with subscript m refers to the model functional representation of output variables as per (7). Additionally, the plant data are collected through measurements vector y_k (9). Notice that, at most y_k vector (measurements) has the same components as y_m at each time instant t. Typically, y_m comprises a larger amount of components, simply due to impossibility or inconvenience of measuring all the properties represented in the model by y_m. We aim to estimate current states given past data over a "sliding time window" [*t-N, t*], then $I_t^{(N)}$ represents the information vector collected (9). Variables w, represented in the model system of Eqs. (8), are considered as disturbances due to various reasons, such as lack of measurements. Subscript '*k*' refers to the time instant of the estimation of that variable within the time window in consideration.

Therefore, the minimization problem of the state estimation could be expressed as per (12)–(15).

$$\min_{\left(\hat{z}_{t-N}, w_N, \ldots, w_k, \hat{p}\ \right)} \left\{ \left\| \hat{z}_{t-N|t} - \bar{z}_{t-N} \right\|^2{}_P + \sum_{i=k-N}^{k} \left\| \Delta w_{k-i} \right\|^2{}_Q + \sum_{i=k-N}^{k} \left\| y_i - y_m(i) \right\|^2{}_R \right\} \tag{12}$$

Such that:

$$z_{lb} \leq \hat{z}_k \leq z_{ub} \tag{13}$$

$$y_{lb} \leq y_m \ \leq y_{ub} \tag{14}$$

$$\Delta w_{lb} \leq \Delta w_k \ \leq \Delta w_{ub} \tag{15}$$

Where R, Q and P are positive definite matrices that weight each term of the cost function. Estimates other than disturbances (w) are represented by a hat accent, such as $\hat{p}$ and $\hat{z}$, for parameters and states estimations respectively. The first term, represents the quadratic arrival cost [18,21,24,25], being $\bar{z}$ the previous estimation of $\hat{z}$. The second term accounts differences of unmeasured disturbances Δw (10) along a time window [*t-N, N*], this term prevents sudden changes in Δw. The third term represents the distance between actual measurements and estimations (7) and (9).

The right hand side of Fig. 12 represents all stages (past and future) in the RTRS on the same timeline. Past data (until *t-N*) is used for the state and parameter estimation of current values (at *t*) of *z, y, w, u*. These are represented by straight lines (continuous functions), and dots (discrete data or estimations). Dashed lines represent the evolution of the system in the future according to the simulation, which is further described in the following section.

As the purpose of MHE is initializing the dynamic simulation in order to perform other studies or evaluations, the MHE is embedded in the simulation environment and the dynamic optimization is performed following a sequential approach. The whole procedure is shown in Fig. 13, which displays the steps

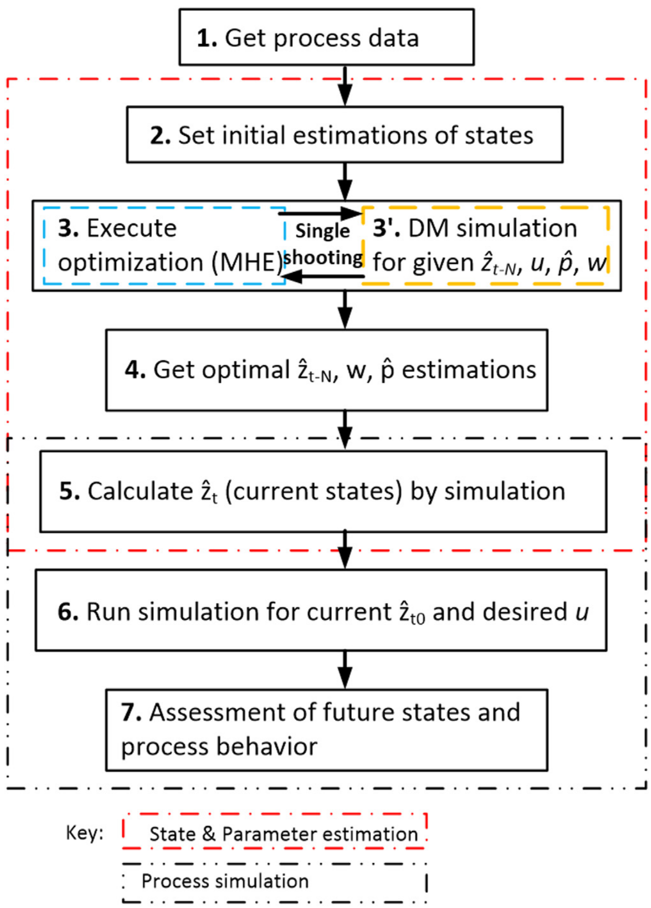

Fig. 13. Generic procedure for the proposed MHE integrated in a simulation framework.

for automatic estimation of current plant states and parameters, followed by dynamic simulation. The conceptual design and architecture presented was first introduced by [26].

Steps 1–2 are required to run a NLP optimization, where $\hat{p}$, $\hat{z}_{t-N}$ and w are the decision variables. Firstly, data are collected from the Process Information system. Then, initial values for decision variables are required for the DAE and NLP solver. It should be noticed that, feasible initial values are required for this method to initialize properly. They can be obtained from the last iteration of the data reconciliation module. Estimations from previous executions or reconciled data records would also provide good initialization points.

Steps 3–3' refer to the optimization itself to determine the states estimations, applying a single shooting sequential approach as described by [27, chap. 9], and represented in Fig. 14. In this case, the gradients of the objective function and constraints w.r.t. $\hat{z}_{t-N}$, $\hat{p}$ and w (decision variables, for short) are determined by the DAE solver computing sensitivities in the DM simulation, and passed on to the nonlinear programming (NLP) solver, as well as the initial values. The NLP solver returns back to the simulation with the decision variables, where the rest of the variables are determined (i.e.: y_m, z), as well as the objective function and constraints in (12)–(15). This runs iteratively governed by the optimization algorithm until reaching optimality tolerance or any other termination point of the NLP solver. This optimization approach has the advantage of embedding naturally in a simulation framework, and therefore, enabling a straightforward execution of the whole process directly from the simulation software. In addition, the optimization problem itself is shrunk to the space of the decision variables alone, being the rest of the variables calculated at the DAE instance for any given decision variables estimated. However, this may as well be a downside of the method, since it does not exploit the full capacity of state-of-the-art NLP solvers for large-scale problems. One broadly used approach to overcome this issue is to apply full space discretization with automatic differentiation, however this kind of method have the disadvantage of weak, if any, embedded capability with simulation environments. A thorough and insightful discussion of advantages and shortcomings of these dynamic optimization approaches, and how they apply to state estimation and optimal control is presented by [27, chaps. 8–9]. This is beyond the scope of this manuscript.

Step 5 takes care of the last stage of the current state and parameter estimation. First, with the decision variables and past controls, a simulation from t-N to t is executed to obtain $\hat{z}_t$ (estimation of current state). Notice that $\hat{p}$, by definition, is time independent, therefore valid and constant for the whole simulation time window, i.e. [t-N, t] while the estimated past disturbances w change over time. MHE ends at this point providing a reliable starting point for the process simulation.

Thereafter, steps 6–7, $\hat{z}_t$ is used as initialization for process forecasting, where the DAE solver is given a set of future u depending on the purpose of the simulation and the set of scenarios considered. These scenarios should be deemed relevant for the case study, assessment, what-if analysis or any other final end of the RTRS.

The implementation of MHE within EcosimPro®/Proosis® [17] takes advantage of its capability of generating C++ classes and linking dynamic-link library (dll) routines in order to integrate and manage other software. The integration of the DAE system corresponding to the model is done with a sparse version of IDAS [28–30], which also provides on-line values of the sensitivities to compute exact gradients for the MHE dynamic optimization. The NLP solver is SNOPT [31,32] as reduced-space NLP solver suitable for sequential optimization.

The system integrator (DAE solver) has to work out all unknown variables, for a given set of boundaries and parameters of the system. Some of these are in turn estimated by the MHE routine within the RTRS procedure, while others are given by the user to represent known boundaries (e.g. ρ_{HC}, MW_{HC}). It is important to notice that, a stream has several variables associated and solving the model means that all of them are either calculated by the DAE solver (i.e. explicit, dynamic) or given by the user (e.g. boundaries). In addition, the RTRS application is providing a means of estimating states (dynamic variables) and parameters, such that plant data vs model mismatch is minimized. In other words, decision variables in the RTRS case studies are initial values at time t-N of states (i.e. $\hat{z}_{t-N}$), model parameters (i.e. $\hat{p}$) and disturbance variables (i.e. w), see Fig. 13.

It is important to notice that, in the proposed scheme signal noise is neglected as plant data is sourced in average form (e.g. 5 min average) from a historian server. In addition, unmeasured disturbances are directly calculated in w. In regards to gross errors, these are not calculated directly in this RTRS formulation for simplicity (it may well be incorporated in the future). Instead, these are accounted indirectly by using off-set values of instrument readings, which are worked out from steady state reconciliation data sourced externally. In this case, this is proven practical because the RTRS is used alongside a previously implemented steady state real-time data reconciliation (DR) tool (revisit Fig. 6). This DR tool provides robust estimations of streams and model parameters in steady state at two-hour time intervals, which are used conveniently to estimate off-set values in instrument readings. Further details of the DR formulation are addressed by [12,13].

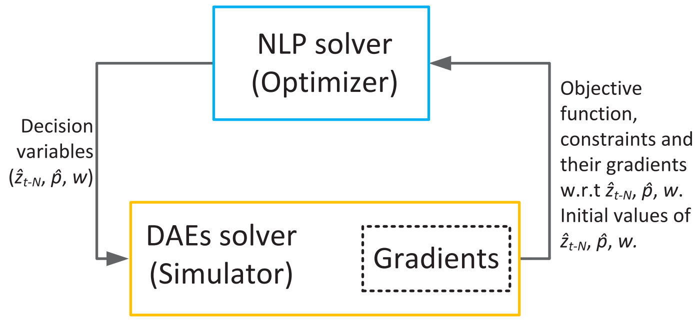

Fig. 14. Representation of single shooting sequential approach used for solving the MHE, i.e.: dynamic optimization problem, for $\hat{z}_{t-N}$, $\hat{p}$, w (decision variables, for short).

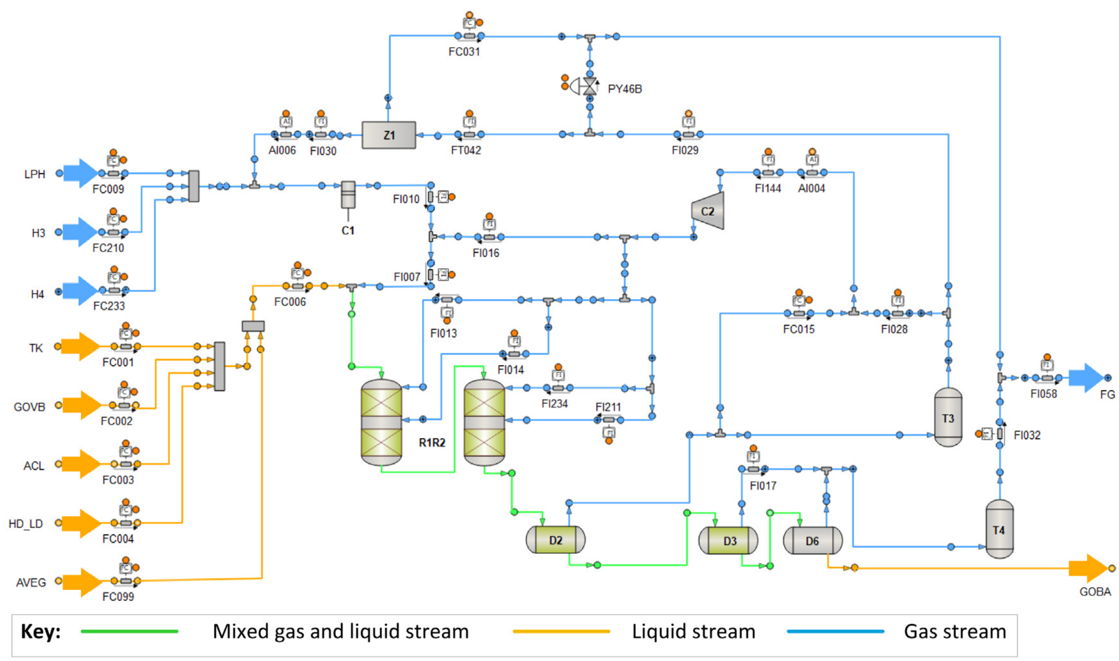

Fig. 15. G3 middle distillate HDS flow diagram developed for RTRS (case I). TK, GOVB, ACL, HD_LD, AVEG are HC feeds from different precedence. H3 and H4 are HPHs of steam reforming units. C1: make-up reciprocating compressor. C2: recycle compressor. R1R2: hydrotreating reactors R1 and R2. D2: high pressure separator. D3: medium pressure separator. D6: low pressure separator. T3: amine absorption column. T4: low pressure off-gas column. Z1: H_2 permeation membrane unit.

4.3. What-if analysis

A scenario-based analysis comes naturally with the idea of simulation, and in this case, RTRS enhances the impact of the analysis by the incorporation of current plant states and parameters. Furthermore, in this study a what-if analysis (WiA) is loosely defined as a scenario-based analysis in which the scenarios represent potential process or machinery degrading conditions. The analysis focuses on the best set of actions for a given scenario, assuming that the decision maker lacks of online information of states and key parameters are unknown or uncertain. Therefore, RTRS makes sense as a decision support tool. In contrast, other scenario-based studies may rely on hazardous process conditions, or even purely normal operation events, mostly based on design or offline historical data, or, in case of the hydrogen network, evaluation of the solutions computed by the RTO module that cover the whole set of plants involved and may indicate better operation decisions than the ones applied by the LP+DMC implementation.

In this context, WiA is used for assessing the usefulness of RTRS applied to case studies. In addition, one of the central features of RTRS is its simplicity, and straightforwardness, towards its integration with the plant information system, and graphic interface. Moreover, the control room schematics can easily be reproduced in the RTRS application, supporting a quick familiarization of operators with the tool.

5. Case studies

Presenting a case study with the whole network as represented in Fig. 11, due to the large number of variables and elements involved, is too complex for the length of a journal paper. Instead, we present two RTRS case studies inspired in actual HDS plants and Petronor crude oil refinery hydrogen network, though for confidentiality reasons either figures or configuration have been modified. In any case, these represent fairly accurately process systems dynamics, which is deemed sufficient for discussing RTRS usefulness as a decision support tool.

Two independent exercises, a plant (case I) and a network (case II), are presented in the framework of refinery hydrogen network case studies. These provide the baselines for analyzing different sets of actions towards process improvements. For this purpose, the impact on *Profit* (as defined in (6)) for each set is accounted. All process units are modeled using the refinery hydrogen library, i.e. HDSLib, representing their actual network

Table 3
Summary of case studies conditions and mitigation sets of actions. *Stream or equipment related to the variable is between square brackets in italics. [*R1R2*]rd_{H2SS} changes from 65 Nm^3H_2/m^3HC to 75 Nm^3H_2/m^3HC @0.2 h.

	Case I (G3 plant)		Case II (Network)	
	Description	Variable*	Description	Variable*
Baseline (BL)	15% H_2 demand increase	[*R1R2*]rd_{H2SS}	5 m^3/h HC load increase (in HDS1)	[*FC001*]*HC*
Violation	Recycle gas purity LL violation	[*AI004*]X_{H2}	Recycle gas purity LL violation	[*AI001*]X_{H2}
Mitigation SA	Membrane feed increase	[*FT042*]*F*	1. HDS1 HPH make-up rise 2. HDS1 HC load decrease	1. [*FI003*]*F* 2. [*FC001*]*HC*
Mitigation SB	HPH make-up increase	[*FC233*]*F*	1. HDS1 HPH make-up rise 2. HDS2 HPH make-up decrease	1. [*FI003*]*F* 2. [*FI004*]*F*

Table 4
Main variables and streams of case I, their tags, description and impact. *Described in Table 1. B: boundary variable. E: explicit variable. D: dynamic variable. P: parameter. OP: output of RTRS. MV: manipulated variable. CV: controlled variable.

Stream/Equipment	Variable	Tag	Description			Impact
TK	HC, ρ, MW	FC001	B	MV	HC load	H_2 and HC balance
GOVB	HC, ρ, MW	FC002	B	MV	HC load	H_2 and HC balance
ACL	HC, ρ, MW	FC003	B	MV	HC load	H_2 and HC balance
HD	HC, ρ, MW	FC004	B	MV	HC load	H_2 and HC balance
AVEG	HC, ρ, MW	FC005	B	MV	HC load	H_2 and HC balance
H3	F, X_{H2}, MW_{LIG}	FC210	B	MV	MU gas	H_2 balance. High impact on purity.
H4	F, X_{H2}, MW_{LIG}	FC233	B	MV	MU gas	H_2 balance. High impact on purity.
R1R2.Q1	F	FI013	B	MV	Quench	Neutral
R1R2.Q2	F	FI014	B	MV	Quench	Neutral
R1R2.Q3	F	FI234	B	MV	Quench	Neutral
R1R2.Q4	F	FI211	B	MV	Quench	Neutral
FI144	F	FI144	B	MV	Recycle	Neutral
FT042	F	FT042	B	MV	Membrane feed	H_2 balance. High impact on purity.
PY46B	F	PY46B	B	MV	High pressure purge	H_2 balance
FC006	HC	FC006	E	CV	HC load	H_2 and HC balance
LPH	F	FC009	E	CV	MU gas	H_2 balance. High impact on purity.
D2.Gas	F		E	CV	Off-gas	H_2 balance. Highly sensitive to ksol changes.
D3.Gas	F	FI017	E	CV	Off-gas	H_2 balance. Highly sensitive to ksol changes.
GOBA	HC		E	CV	Product	HC balance
AI004	X_{H2}	AI004	E	CV	H2 analyzer	H_2 balance. Purity control point.
FI016	F	FI016	E	CV	Recycle tie-in	Neutral
FI030	F	FI030	E	CV	Membrane effluent	H_2 balance
AI006	X_{H2}	AI006	E	CV	H2 analyzer	H_2 balance
FC031	F	FC031	E	CV	Membrane purge	H_2 balance
FI032	F	FI032	E	CV	Off-gas	H_2 balance
FI058	F	FI058	E	CV	Plant vent	H_2 balance
LPH	F	FC009	E	CV	MU gas	H_2 balance. High impact on purity.
R1R2	HC_{out}		D	OP	*	HC and H_2 balance
R1R2	rd_{H2}		D	OP	*	H_2 demand. High impact on recycle purity.
R1R2	rd_{LIG}		D	OP	*	LIG generation
D2	HC		D	OP	*	HC and H_2 balance
D2	$ksol_{H2HC}$		D	OP	*	Recycled H_2 and losses to FG.
D2	$ksol_{GASHC}$		D	OP	*	Recycled gas and losses to FG.
D3	HC		D	OP	*	HC and H_2 balance
D3	$ksol_{H2HC}$		D	OP	*	H_2 losses to FG
D3	$ksol_{GASHC}$		D	OP	*	Gas losses to FG
R1R2	rd_{H2SS}		P	OP	*	Steady state H_2 demand
R1R2	rd_{LIGSS}		P	OP	*	Steady state LIG generation
R1R2	tau		P	OP	*	Time to steady state
D2	$ksol_{H2HCSS}$		P	OP	*	Steady state recycled H_2 and losses to FG
D2	$ksol_{GASHCSS}$		P	OP	*	Steady state recycled gas and losses to FG
D2	tau		P	OP	*	Time to steady state
D3	$ksol_{H2HCSS}$		P	OP	*	Steady state H_2 losses to FG
D3	$ksol_{GASHCSS}$		P	OP	*	Steady state gas losses to FG
D3	tau		P	OP	*	Time to steady state
LPH	X_{H2}	FC009	P	OP	*	H_2 balance. Disturbance.
R1R2	MW_{LIG}		P	OP	*	Product density. Disturbance.

setting. Fig. 15 shows the schematic of G3, the plant selected for case I, as it is represented for RTRS.

In contrast, case II is based on three typical HDS plants and their corresponding hydrogen network configuration across a refinery. Rather than an actual process network, case II is a simplified representative example aimed at demonstrating RTRS usefulness at network level. Hydrogen network with the three plants and a detail of the internal configuration of the HDS plants are presented in Figs. 16 and 17 respectively.

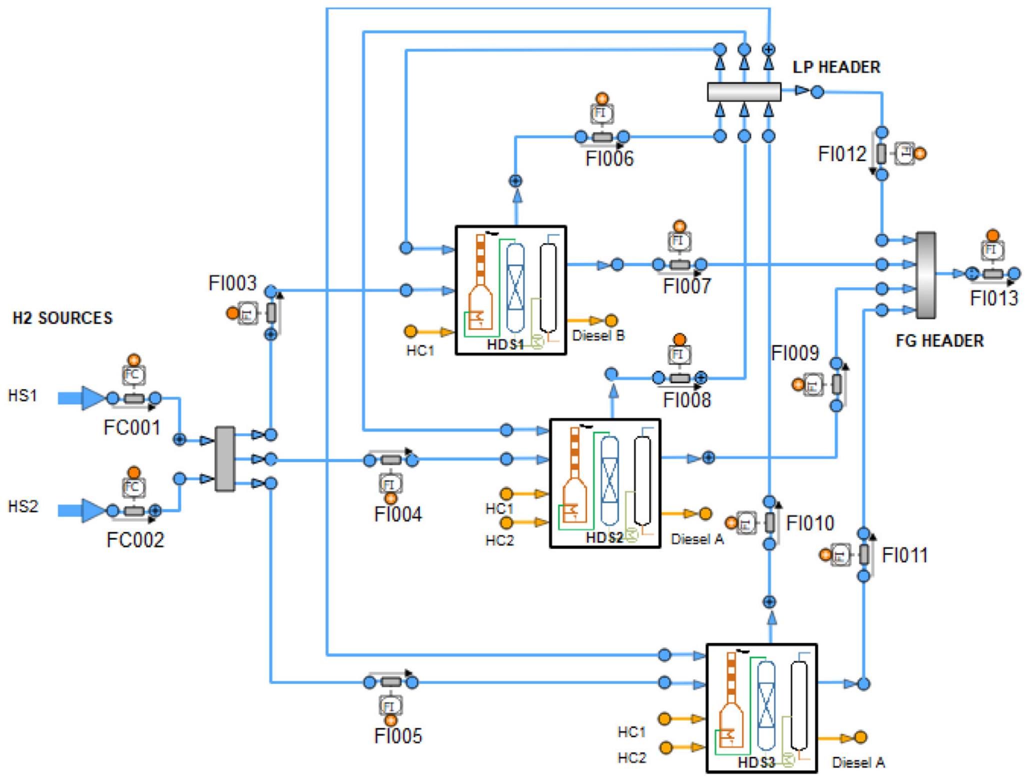

Fig. 16. High level schematic of hydrogen network (case II). Two hydrogen sources: HS1 and HS2. One low purity header (LPH), aimed at collecting plant's recycle loop purges and feed them back to the process make-up. One fuel gas header (FGH), aimed at collecting gases from low and medium pressure separators at plant level, and LPH purge.

Table 5
Main streams of case II at network level, their tags, description and impact. *Described in Table 1. B: boundary variable. E: explicit variable. D: dynamic variable. P: parameter. OP: output of RTRS. MV: manipulated variable. CV: controlled variable.

Stream/Equipment	Variable	Tag	Description			Impact
HS1	F, X_{H2}, MW_{LIG}	FC001	B	MV	HPH Source	H_2 balance and purity.
HS2	MW_{LIG}	FC002	B	MV	HPH Source	Gas balance.
FI003	F	FI003	B	MV	MU gas to HDS	H_2 balance and purity.
FI006	F	FI006	B	MV	Purge to LPH	H_2 balance and purity.
FI008	F	FI008	B	MV	Purge to LPH	H_2 balance and purity.
FI010	F	FI010	B	MV	Purge to LPH	H_2 balance and purity.
FI004	F	FI004	E	CV	MU gas to HDS	H_2 balance and purity.
FI005	F	FI005	E	CV	MU gas to HDS	H_2 balance and purity.
FI007	F	FI007	E	CV	Purge to FGH	H_2 balance and purity.
FI009	F	FI009	E	CV	Purge to FGH	H_2 balance and purity.
FI011	F	FI011	E	CV	Purge to FGH	H_2 balance and purity.
FI012	F	FI012	E	CV	LPH to FGH	H_2 balance and purity.
FI013	F	FI013	E	CV	FGH off-gas	H_2 balance and purity.
HS2	F, X_{H2}	FC002	E	CV/OP	HPH Source	H_2 balance and purity.
HDS1.AI001	X_{H2}	AI001	E	CV	*	H_2 balance. Purity control point.
HDS2.AI001	X_{H2}	AI001	E	CV	*	H_2 balance. Purity control point.
HDS3.AI001	X_{H2}	AI001	E	CV	*	H_2 balance. Purity control point.

5.1. Actions assessment description

For each case study (I and II), a What-if analysis (WiA) based on three sets of actions is presented, these are: baseline (BL), actions A (SA) and actions B (SB). The baseline set, represents the process variables before and after a change of condition, without any additional corrective actions from the operators, where at least one operational constraint is not satisfied. Therefore, this is the WiA input, giving meaning to the analysis by setting a constraint violation situation. While, SA and SB are, independent feasible operation strategies proposed by an operator applying RTRS, aimed at mitigating undesirable change of conditions. Table 3 summarizes the main features of each case study: baseline conditions, impact on constraints and analyzed sets of actions for mitigation.

In addition, a qualitative analysis of the main streams and variables of case I is presented in Table 4. These include descriptions of those variables and their main impact in the process and its economy. Variables fall into one of the following groups: manipulated variables (MV), controlled variables (CV), disturbance variables (DV) and measurements. At the same time, MV are boundaries of the system, while CV are explicit variables. Moreover, decision variables of the RTRS are identified as outputs (OP) in the variables' list.

Essentially, the analysis is focused on determining, the system state from plant data and simulating suitable mitigation sets of actions (SA and SB) by running a RTRS application. For didactic purposes a reduced set of variables (see Table 3) is presented in the analysis, however, in actual practice RTRS users

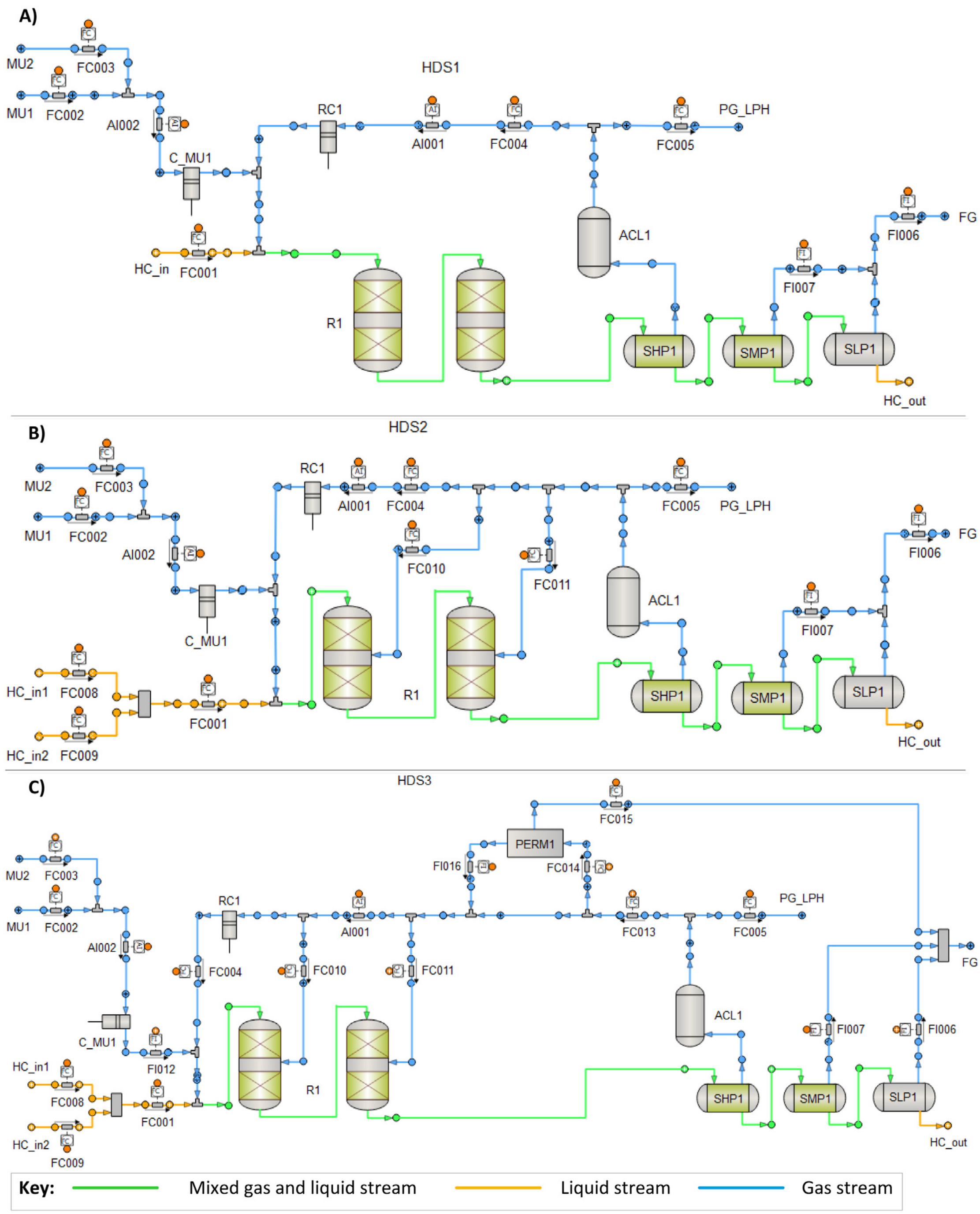

Fig. 17. Flow diagrams of case II, hydrogen consumers, i.e.: HDS1-3. (A) HDS1. (B) HDS2. (C) HDS3.

are encouraged to consider all potential variables in the analysis. This approach is intended to support operators in their decision-making process, such that a negative change of condition is mitigated in the most cost-effective way, considering *Profit* and process specification.

Case II has a homologous set of streams to case I at unit level, with the addition of network streams to interconnect all plants. Thereby, Table 5 presents key variables at network level and their descriptions, rather than a full list, in the interest of conciseness.

A summary of statistics of both models is shown in Table 6. These are intended to provide a broad idea of the size of the models in question.

5.2. Assessment of the accuracy

Even before studying the results of the RTRS at any given condition it is important to assess the accuracy of the estimation during change of conditions, either manual changes or unexpected. In addition, the values in P, Q and R of Eq. (12) are adjusted in order to properly set up the parameter and state estimation module. This task requires some level of judgment and knowledge of the process towards which variables "tighten" more than others in the formulation. For instance, purity readings in the recycle loops are key in getting good estimations, while these are the ones that present more erratic readings or discrepancies. Similarly, some gas flowrates are also critical in resolving the system, e.g. recycled gas from separators, however not all process

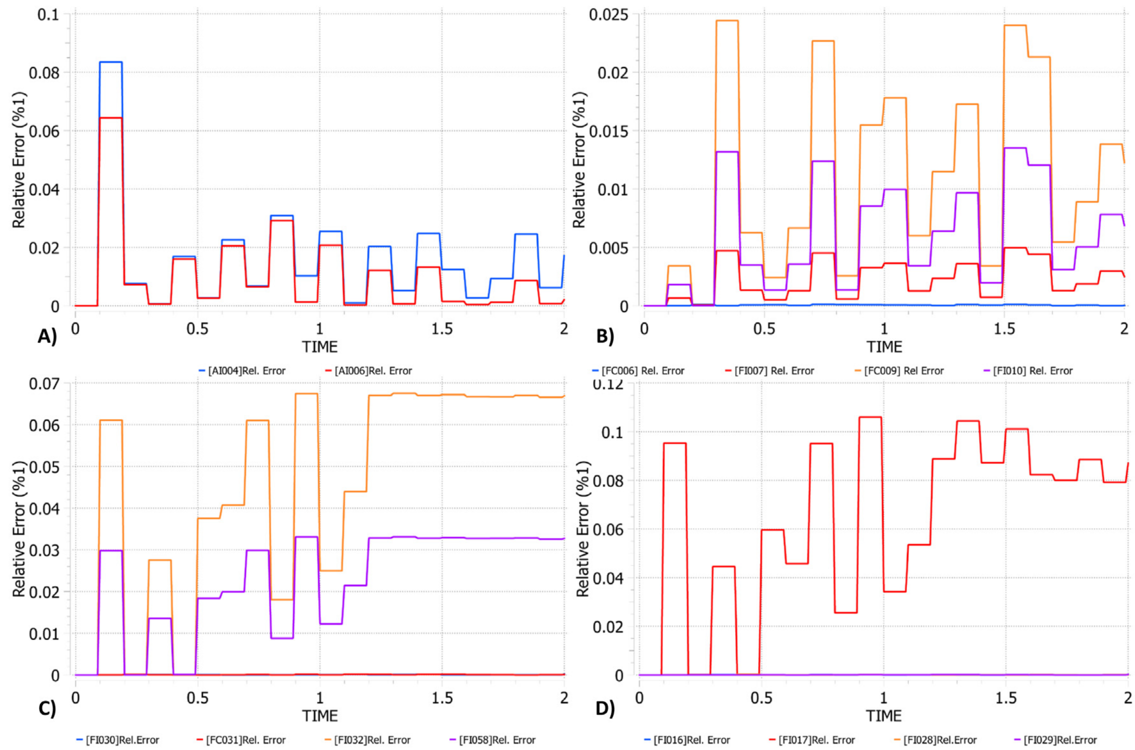

Fig. 18. Case study A (G3) accuracy of parameter and state estimations. A, B, C and D, present the relative error (%*) of online measurements over time, compared to the estimations computed by RTRS tool. *Estimation error over actual value in %.

Table 6
Summary of models' characteristics.

Description	Case I	Case II
Equations	645	1305
Boxes (coupled subsystems of equations)	3	5
Linear boxes	2	4
Nonlinear boxes	1	1
Input DATA	290	592
Output EXPLICIT	634	1273
Output DYNAMICS	9	27
Output ALGEBRAICS	2	5
Size of Jacobian matrix (DYNAMIC+ALGEBRAIC).	11 × 11	32 × 32
Integration method	IDAS	IDAS

units have readings in this section. In the end, tuning the state estimation is a balancing act to make the best estimations at reasonable computation costs. First and foremost, predictions are to be useful if the estimations are within a sensible uncertainty range. Although a detailed study of the accuracy of the estimations and MHE calibration is outside the scope of this manuscript, a brief conceptual description is provided along with relative errors (w.r.t. actual values) of key variables tested for G3 (Case I) shown in Fig. 18.

Starting from reconciled values of the process, the RTRS is executed offline altering a number of variables such as hydrogen demand, hydrogen purity, HC load, among others. The test consists of simulating several changes in operating condition, both expected and unexpected, for a 2 h period of time. In this way, true values are known beforehand and used for calculating the relative error of variables. Simultaneously, the state estimation block of RTRS is run continuously, outputting estimates of states and parameters. In this way, the MHE is qualitatively validated, prior to its online use for any particular process unit. The main purpose of this validation is to adjust the state estimation routine to calculate values within reasonable error ranges. These results are shown in Fig. 18, quadrants A to D.

The state and parameter estimation block of the RTRS presents satisfactory results in terms of estimation accuracy of the method. The most remarkable outcome is probably that, even though errors vary widely across variables most of the errors are below 10% which is considered satisfactory in this type of gaseous industrial networks. Naturally, the more accurate the better, however these figures should only be taken as a first safe reference for validation of the estimations. Adjusting values in R (12) is possible to relax or tighten the error for each measurement in the MHE block (estimation error over actual value in %). Moreover, it is pointed out that key instrumentation should receive greater weight in R in order for achieving the best results. In overall, the estimation itself is considered validated for the purpose of this study. Actual applications should undergo a rigorous validation process which would be fit for purpose, rather than following a general validation criteria. A detailed study of these aspects of the proposed methodology and analysis of the tuning process is out of the scope of this work.

It is important to bear in mind that sensible estimations are essential for further state predictions, and plant forecasting. Estimations of future variables, relies on current time estimations. Therefore, a thorough tuning process is advised during commissioning of any RTRS tool.

5.3. Results and discussion

Even though a discussion based on the results of the WiA is given for each scenario and case study, the focus is on the methodology and tool purpose, i.e. RTRS, rather than a detailed analysis of all process variables and constraints which is out of the scope of this study. For this reason, only the main affected variables' results are presented, in order to analyze the method potential as decision support tool for operators.

RTRS is run on a PC Intel®Core^{TM} i7-6500U CPU at 2.50 GHz RAM 16 GB, and takes 26 s and 40 s on average for Case A and

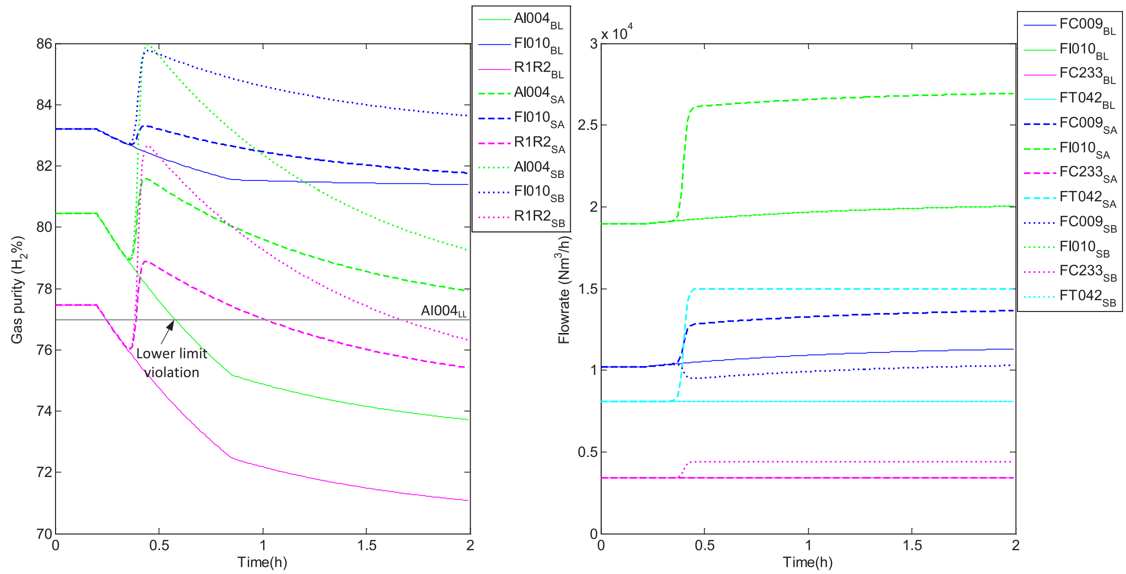

Fig. 19. G3 main variables computed at BL, SA and SB. Left, gas purities of streams: recycle gas (AI004), aggregated make-up and purified gas (*FI010*) and reactor effluent (*R1R2*). Lower limit violation is pointed with an arrow (*AI004$_{LL}$*). Right, gas flowrates of streams: LPH make-up gas (*FC009*), aggregated make-up and purified gas (*FI010*), HPH make-up gas (*FC233*) and membrane feed (*FT042*). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 7
Prices and costs considered for the economic valuation of scenarios (6).

	Description	Case I	Case II
pr_i (k€/m^3)	Price of HC produced of quality *i*, i.e.: Diesel A, Diesel B and GOBA. Represents increase of profit in the process economy balance (6). The same price is used across HC qualities.	1	1
$ct_{\mathrm{HS,i}}$ (k€/Nm^3)	Cost of high purity hydrogen supply of source *i*. Represents loss of profit in the process economy balance (6). Two high purity hydrogen sources are used across cases (i = 1, 2).	1.5E−3, 2.0E−3	1.5E−3, 2.0E−3
$ct_{\mathrm{LPH,i}}$ (k€/Nm^3)	Cost of low purity hydrogen supply of source *i*. Represents loss of profit in the process economy balance (6). One source of LPH is used across cases (i = 1).	1E−4	1E−4

B respectively, per sample time to complete the execution. In addition, costs and prices used in (6) are shown in Table 7. It is worth mentioning that, prices and costs are representative rather than real for confidentiality reasons.

5.3.1. Case I: RTRS at plant level

This case study is an example of RTRS at plant level (G3 process unit, Fig. 15). Baseline (BL) process conditions represent an unexpected 15% increase in rd_{H2SS} (H_2 demand per volume unit of feed) at 0.2 h (see Fig. 16), these change of condition is a consequence of plant feed becoming richer in sulfur components. Moreover, it impacts on the recycled gas purity (*AI004*, Fig. 19 - left) resulting in a significant drop of this controlled variable. Recycle gas purity lower limit (LL), 77% H_2, is violated after the change in H_2 demand realizes, requiring an action from the operator. In this context, SA shows the effect of increasing the purification membrane load (*FT042*, Fig. 19 - right). SB presents the impact of using HPH make-up feed instead (*FC233*, Fig. 15 - right). Note that in Fig. 19 three different purities are portrayed (AI004, FI010 and R1R2), however the process constraint (lower limit) is only imposed on AI004 (in green in Fig. 19) as this is the only actual plant reading.

Certainly, it has to be noticed the fact that for both sets of actions profit is lower than for BL. This is explained due to an increase in H_2 demand in reactors (*R1R2*, which rises make-up gas demand. Thereby, hydrotreating costs are higher producing the same amount of low sulfur product. For instance, this would be the case when crude oil tanks are changed or HC feed streams change their composition for any other reason.

It is seen that, although both SA and SB are effective mitigation actions, towards steering the process within recycle gas constraint (Fig. 19 – left), SA provides the most cost-effective response outweighing SB strategy by around 47% (Fig. 20). This results show the key importance of purification units for addressing the best possible operation. It must be borne in mind that, membranes are rarely operated automatically from the control room, instead, are likely to require manual intervention from a field operator. This is exactly the case of G3 process unit. Therefore, this analysis is valuable as a training example for operators, as well, for it quantifies actual impacts of different mitigation alternatives (Fig. 20). In particular, presenting that is better to address H_2 demand changes at plant level by manipulating the purification membrane rather than make-up gas. This results are in line with previous finding presented by [16], where a focus on the optimum H_2 management policy is addressed showing the importance of membranes operation.

5.3.2. Case II: RTRS at network level

This case study shows an example of RTRS at network level. BL, presents a H_2 demand increase due to a HC load rise by 5 m^3/h (3.2%) in HDS1 (*FC001*, Fig. 21 - right), decreasing recycle gas purity of HDS1 below its lower limit (see *AI001* in Fig. 18 - right), 68% (*AI001$_{LL}$*), requiring an action from the operator. In this context, SA shows the effect of manipulating HPH make-up (*FI003*, Fig. 21 – left) and *FC001*, being both mitigation actions

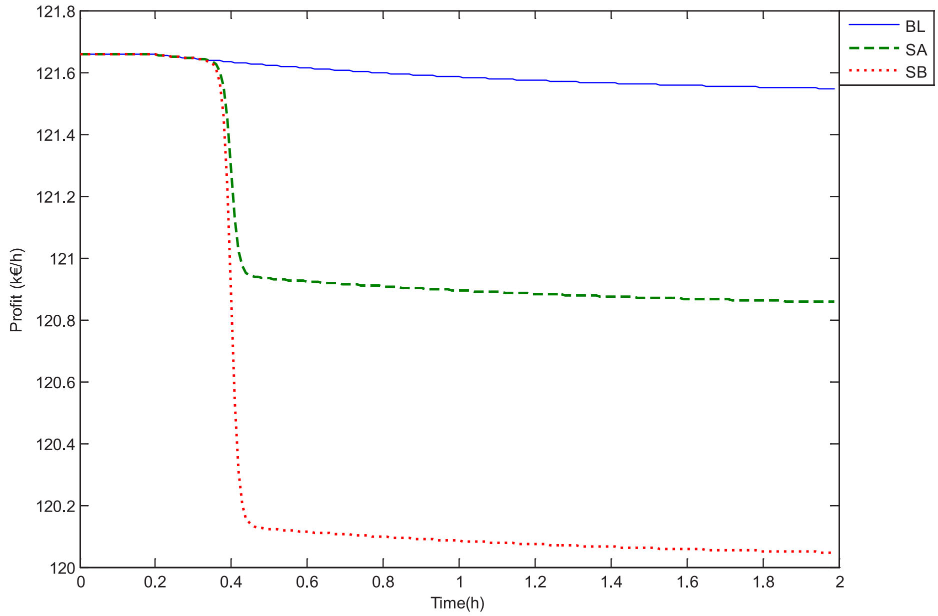

Fig. 20. G3 process profit, in k€/h at all scenarios. Profit does not consider operational constraints (14), such as gas purity in reactors. Values are representative rather than actual for confidentiality reasons.

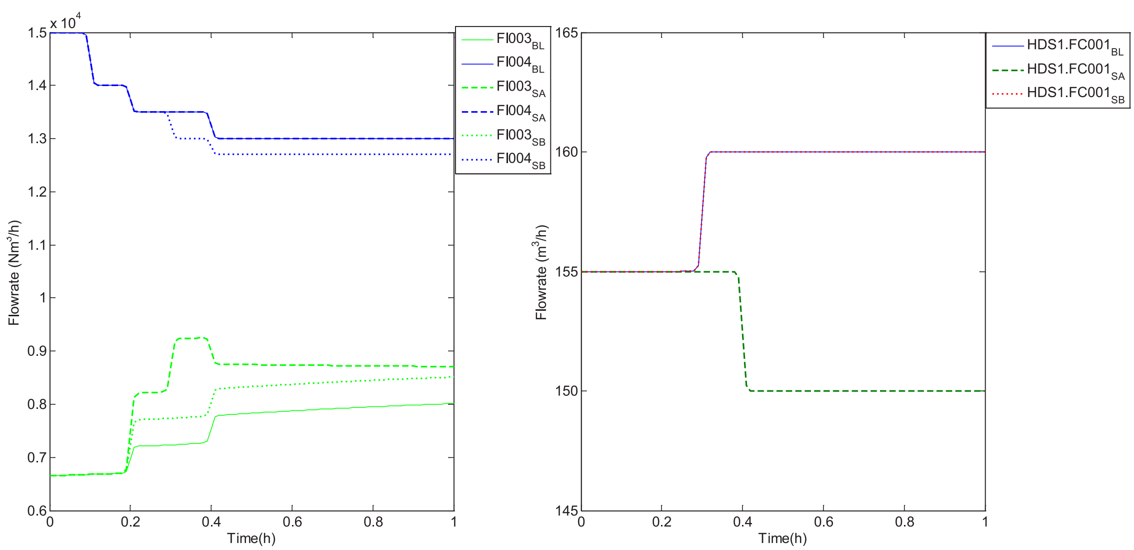

Fig. 21. Left: HPH make-up gas streams *FI003* (HDS1) and *FI004* (HDS2) in Nm^3/h. Right: HDS1 hydrocarbon load (*FC001*) in m^3/h.

local to HDS1. On the other hand, SB shows corrective actions manipulating HPH make-up in HDS1 and HDS2 (*FI004*, Fig. 21 – left), being a network-wide strategy.

In this case, SA and SB satisfy the recycle gas purity constraint after time 0.2 h, therefore are both deemed to be corrective actions (Fig. 22 – right). However, it is observed a significant negative impact on *Profit* of SA compared to SB (Fig. 23 – right). The reason for this is that SB copes with HC load changes by purely rearranging H_2 distribution across the network. Concretely, cutting back H_2 feeding HDS2, allowing more make-up to HDS1 (Fig. 21 - left). Therefore, impact on process economy is minimized in the sense that production is not reduced. However, SA strategy applies only HDS1 local MVs to mitigate the change of condition, taking a toll on process economy. Moreover, it does not reach the production level of 160 m^3/h as required (*FC001*, Fig. 21 - right). An interesting outcome to point out is that, an operator would rather manipulate variables within his process unit boundaries, not considering the impact of actions in other process units in the network. In this case, it is clear how that approach is not the best possible, presenting an alternative that enables an increased HC load while keeping constraints within limits. Even more, this is an example of how network interactions between plants are key elements for troubleshooting. And RTRS demonstrates its usefulness for addressing this sort of challenges.

It must be pointed out that building models at network level is more complex than at plant level. Similarly, the analysis of results and their interpretation requires more knowledge. Thereby, it is sensible to assume that RTRS at network level should be a useful tool for experienced operators or supervisors, while might seem not easy to build up meaningful sets of actions or scenarios for novice operators. Still, for training purposes it should be valuable as well.

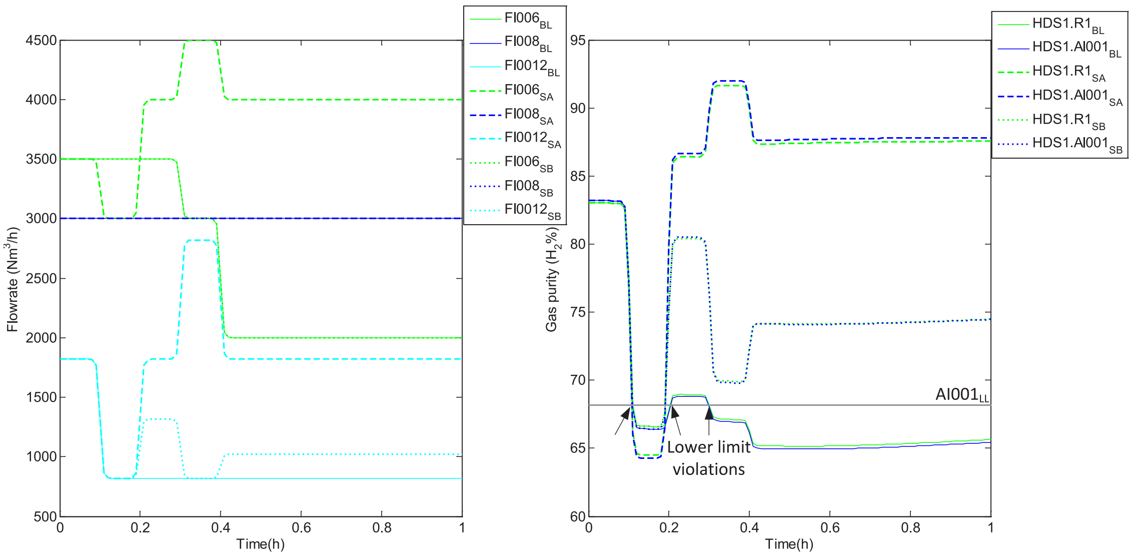

Fig. 22. Left: LPH streams in Nm^3/h. Right: HDS1 recycle (*AI001*) and reactor effluent (*R1*) gas purities in H_2%. Lower limit violations are pointed with arrows ($AI001_{LL}$).

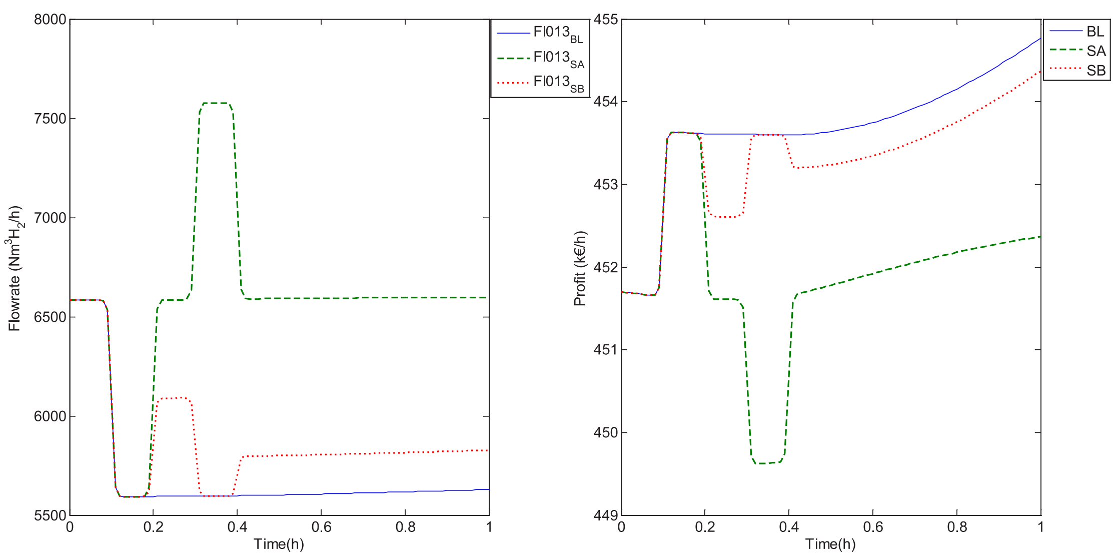

Fig. 23. Left: gas flowrate to FGH (*FI013*) in Nm^3 H_2 /h. Right: process profit in k€/h (14).

5.3.3. General highlights

RTRS methodology has significant versatility, due to its capability of adaptation to several purposes such as analysis based on predefined sets of actions or training. For instance, this paper showcases WiA based on RTRS at two levels in a process network (plant level and network level). Moreover, RTRS presents especial interest as a decision support tool for analyzing mitigation actions due to change of condition. Additionally, control room schematics can be replicated on the RTRS graphic interface for ease of understanding and effective communication of outcomes throughout the organization.

Other favorable accountability of RTRS is its complementarity to model predictive control (MPC) and real-time optimization (RTO) layers. Particularly if those are considering the same process system, for example in a refinery H_2 network the integration would be MPC, RTO and RTRS. MPC and RTO would take care of actual closed-loop control and economic optimization, while RTRS may contribute providing an analysis tool for better understanding and testing of RTO and MPC solutions. Thereby, it might be the case where operators come up with a set of actions with similar impact on profits than RTO, though easier to perform due to model limitations for representing all constraints and casualties. In this dimension, RTRS complements other existing decision-making and control tools in the process industry. However, this aspect requires further exploration, in order to solve interactions of the different tools with ease. Being the ultimate, ideal, aim to efficiently integrate digital information from: process models, business indicators, maintenance monitoring and supply chain, into a decision support framework.

Another advantage of RTRS is its intuitiveness, since it is based on well-known techniques (MHE and DAEs computation). Hence, RTRS is relatively easy to replicate and develop for any given dynamic process system. Nonetheless, it could be challenging for systems with complex dynamics, if a previous appropriate components library is not available.

In spite of all the previous comments, there are RTRS current limitations to point out as well. Firstly, it is duly noted that single shooting optimization approach has limited effectiveness for handling path constraints or unstable solutions. This shortcoming should be considered in future work, exploring strategies

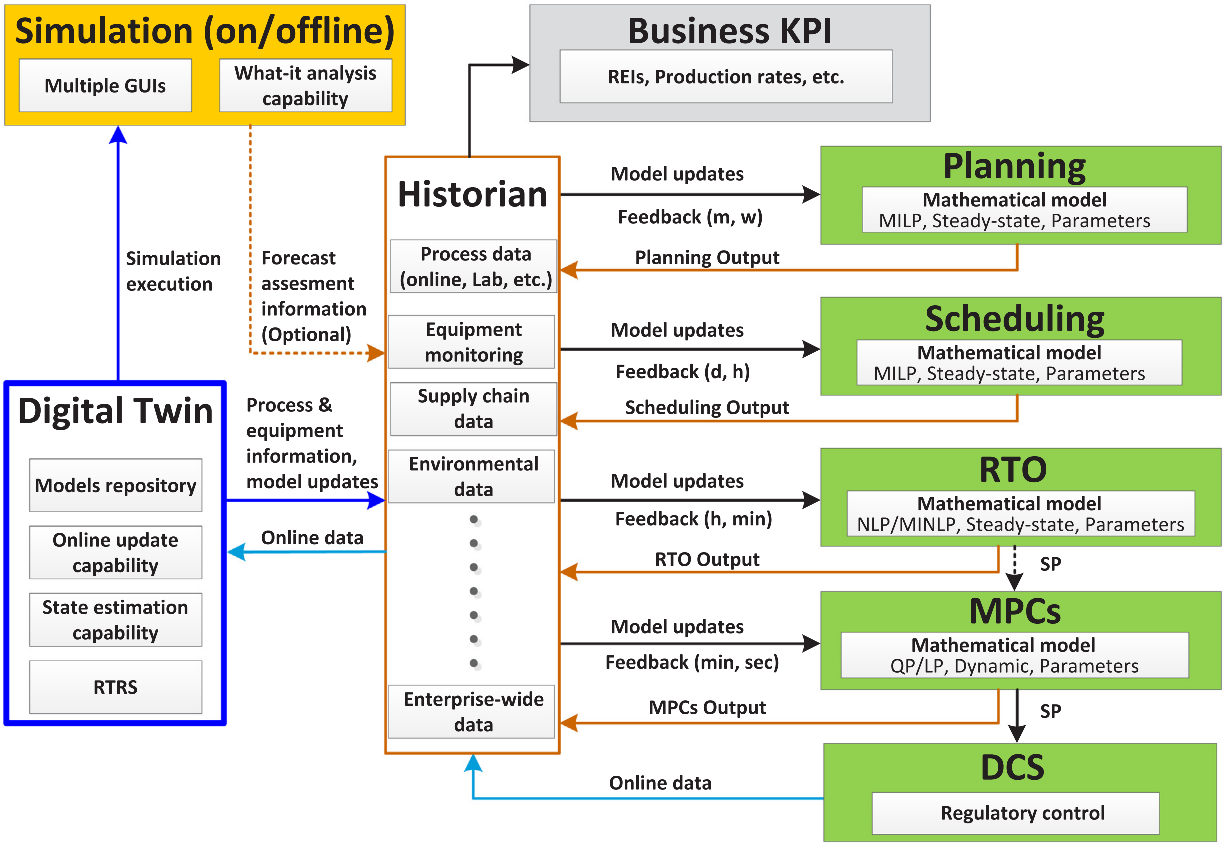

Fig. 24. Example of decision support framework architecture with integration of control layers, simulation and optimization features. REI: resource efficiency indicator. KPI: key performance indicator. DCS: distributed control system. RTO: real-time optimization. MPC: model predictive controller. GUI: graphic user interface. SP: set points. QP: quadratic programming. LP: linear programming. NLP: nonlinear programming. MILP: mixed integer linear programming. MINLP: mixed integer nonlinear programming. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

for automatic finite elements orthogonal collocation and differentiation within a simulation framework. Secondly, RTRS itself is unlikely to provide optimum solutions and run in open-loop, which is generally speaking a downside that comes alongside and at the cost of versatility. However, pairing RTRS with RTO/MPC applications should partly compensate this aspect as mentioned before.

5.3.4. *RTRS use in decision support frameworks*

Decision support frameworks (DSF) with effective integration of RTO, MPC, DCS and RTRS (amongst other decision-making tools), can help decision makers of process operations towards steering processes in the best direction possible. Certainly, this capability depends not only on each individual tool in the DSF, but also on the DSF architecture itself. Therefore, an example of DSF architecture is shown in Fig. 24, which includes all the major players in a DSF envisioned by the authors and how these are linked together. This may help understand in a more general form, the key role of RTRS with respect to digital twins and decision support in process operations.

The proposed decision support framework architecture centralizes data management, easing integration of applications and information exchange between levels as well as within same levels in the control pyramid. For instance, planning, scheduling, RTO, MPCs and DCS are of particular relevance in understanding information exchanges across the DSF and its architecture, since these have several levels of hierarchical dependency with data being managed directly between applications. For example, Fig. 24 depicts a DSF configuration including simulation, optimization and control features, which utilizes a centralized data management system using plant historian database. In addition, the proposed architecture in Fig. 24 incorporates simulation and business KPI features to unleash the full potential of the DSF in aiding decision-making in process operation environments. In the following paragraphs, the architecture is described further, focusing on how this enables seamless information and data exchange across individual applications enhancing decision-making capability.

Firstly, the historian plays the role of the data management system centralizing all sources of data, such as online process measurements, lab data, equipment monitoring data, and others (see Fig. 24). Furthermore, the historian collects key information (outputs) from traditional control and optimization applications (see green boxes in Fig. 24). These outputs are used automatically or on demand by other applications via historian, automated updates follow the feedback frequency required by each application (see feedback arrows in Fig. 24). In this architecture the historian is critical in keeping one data and information repository, which serves client applications requesting those data.

Secondly, the proposed architecture features a digital twin application, which is the root source of models of multiple natures (models repository in Fig. 24). In practice, operates as the library of models concerned to the decision support framework, especially those used in control and optimization tools (see green boxes in Fig. 24). Additionally, the digital twin itself executes automatic state estimation and model update routines using online data pulled from the historian. In fact, the RTRS would be considered within digital twin features to some extent, because it integrates state estimation with real-time simulation as previously discussed. Model updates, estimations and process equipment

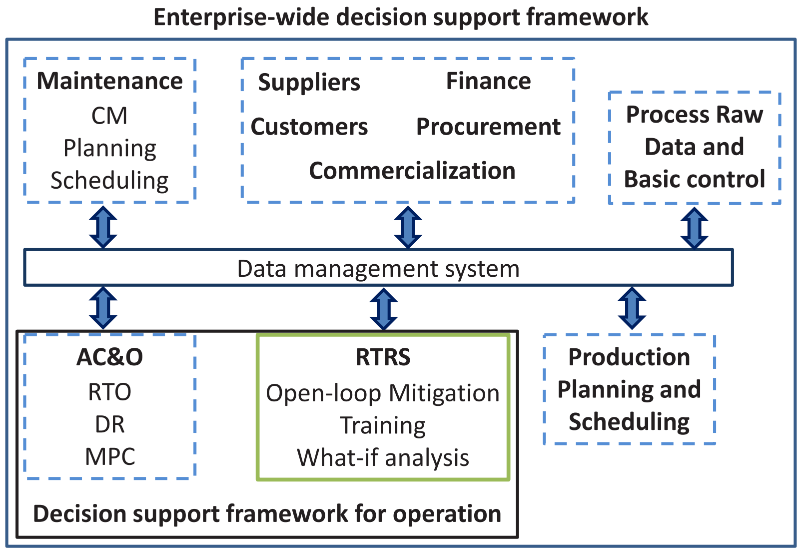

Fig. 25. Enterprise-wide decision support framework, with RTRS highlighted in green. AC&O: advanced control and optimization. CM: condition monitoring. DR: data reconciliation. RTO: real-time optimization. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

information resulting from the digital twin are available for all client applications within the DSF via historian. This architecture helps manage multiple mathematical models since these have the same source which simplifies consistent maintenance and human resource allocation for models maintenance.

Thirdly, this architecture features online and offline simulation with multiple graphic user interfaces (GUIs) and What-if analysis capability (see yellow box in Fig. 24). Users with different profiles can access multiple GUIs which allow them to run simulation experiments via digital twin. GUIs should be assigned to users' profiles to reflect security clearance across users. For example, control room operators should have access to GUIs which replicate DCS dashboards, while process engineers may have clearance to more detailed schematics (including chemical composition of streams, catalyst information, etc.). From GUIs, real-time simulation experiments can be run based on online current data, and RTRS. This provides enhanced forecasting capabilities, which generates results that can be available across the DSF, if necessary (see forecast assessment information, dashed arrow in Fig. 24). Additionally, control actions and other changes can be assessed using What-if analysis capabilities. For instance, optimization outputs from the RTO can be tested in search for simpler control action alternatives from an operating viewpoint with similar results in terms of economic outcome (objective function).

Finally, business indicators are received via historian (see gray box in Fig. 24) in the Business KPIs feature, which help manager and executive level decision makers follow critical business trends with respect to process operations. This module comprises simple visualization tools such as dashboards and KPI charts.

In overall, there are multiple forms for RTRS to support decision-making processes in manufacturing operations, although this may require thoughtful DSF architectures to make the most out of each individual tool.

6. Conclusions

A real-time reconciled simulation tool is presented, aimed at aiding process network operators in their decision-making process, especially under changing plant conditions. RTRS effectively combines dynamic state estimation techniques (MHE) into a simulation environment, which enables both: online data pulling from plant information systems and input of manipulated variables for assessing future conditions. In this context, RTRS is a general concept and virtually applicable to any process network supported on a FPM, given a dynamic library of components is available.

In order to evaluate the usefulness of RTRS as a decision support tool for operators, a what-if analysis approach is conducted on two case studies: an individual process unit (case I) and a process network (case II). Case study I, consists in a real plant of Petronor refinery, studied for a baseline condition where hydrogen demand increases by 15% unexpectedly. Two corrective sets of actions are considered for mitigation (SA and SB) and assessed over their economic impact. It is demonstrated that SA is advantageous over SB, due to a more efficient use of hydrogen purification membranes available in G3. In addition, state and parameter estimation results are presented for case study I, showing a satisfactory accuracy for all key instruments with a relative error below 10%. Case study II, consists in a representative hydrogen network, studied for baseline condition where one process unit faces an increase in hydrogen demand due to an ramp-up in hydrocarbon load. It is shown that set of actions SB is a better mitigation action, due to a more efficient hydrogen management across the network rather than at plant level.

Generically speaking, RTRS methodology is promising for: its versatility of application and ease of communication, complementarity with current plant-wide control systems (RTO/MPC) and intuitiveness of implementation. On the contrary, absence of optimal mitigation actions guarantee and single shooting sequential optimization, are identified as challenges to overcome.

Two additional points are mentioned: one refers to the requirement of the simulation framework of having an HMI able to deal efficiently with thousands of variables and present clear and elaborate information to the users. The other one is the central role played by the process information system (historian), even if this is not a problem in most process industries where a real-time data base like PI is in operation and digitalization takes place since many years ago.

RTRS has being presented as part of a decision support and operation framework around MES and MPC layers, in particular, a DSF example of architecture is presented and briefly described. The roles of RTO, MPC, RTRS, Historian, Digital Twin, amongst other tools, are discussed highlighting why the proposed configuration adds value to the decision-making process. In addition, RTRS can be visualized in a wider perspective as an enterprise-wide decision support framework that includes, for instance, supply chain and production scheduling, machinery condition monitoring and maintenance, to mention only two. In this way, RTRS would take advantage of the most accurate data of machinery performance, or scheduled maintenance when estimating parameters and forecasting future process conditions. Similarly, current time estimations from RTRS may be available in real-time for scheduling and updating data for supply chain operations (Fig. 25). All relevant data from modules within the framework is exchanged through a data management system capable of storing historical data, as well as accessible form several platforms for data search. It is strongly believed, that the integration of tools such as RTRS with other decision-making modules across a business should enhance decision support potential at all levels enterprise-wide. Hence, there is growing interest from process industries in these applications in their transit towards fully digitalized businesses, where digital twins play a central role.

Models play a critical role in nearly all decisions as they have different characteristics and complexities, but they should be kept up to date to be used in real-time when needed. Furthermore, in order for models to be successful these should be coherent and compatible with respect to its scale and purpose. In the paper we have highlighted the importance of RTRS enterprise-wide integration with other modular decision support tools. Models, combined with other tools for prediction, analysis and optimization form the core of modern digital twins. Enabling fully interconnected information at all levels, is likely to bring added value to everyone involved and a step forward in the path towards a wisely applied digital twin approach, which is a fruitful line of future research.

CRediT authorship contribution statement

Anibal Galan: Conceptualization, Formal analysis, Investigation, Methodology, Validation, Writing - original draft. **Cesar De Prada:** Supervision, Project administration, Resources, Funding acquisition. **Gloria Gutierrez:** Software, Supervision, Formal analysis, Data curation. **Daniel Sarabia:** Software, Data curation, Writing review. **Rafael Gonzalez:** Resources, Formal analysis, Writing review.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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References

[1] C. de Prada, D. Sarabia, Data pre-treatment, in: Resource Efficiency of Processing Plants, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2018, pp. 181–210, http://dx.doi.org/10.1002/9783527804153.ch8.

[2] L.T. Biegler, Advanced optimization strategies for integrated dynamic process operations, Comput. Chem. Eng 114 (2018) 3–13, http://dx.doi.org/10.1016/j.compchemeng.2017.10.016.

[3] P. Daoutidis, J.H. Lee, I. Harjunkoski, S. Skogestad, M. Baldea, C. Georgakis, Integrating operations and control: A perspective and roadmap for future research, Comput. Chem. Eng 115 (2018) 179–184, http://dx.doi.org/10.1016/j.compchemeng.2018.04.011.

[4] R. Amrit, J.B. Rawlings, L.T. Biegler, Optimizing process economics online using model predictive control, Comput. Chem. Eng 58 (2013) 334–343, http://dx.doi.org/10.1016/j.compchemeng.2013.07.015.

[5] M. Ellis, H. Durand, P.D. Christofides, A tutorial review of economic model predictive control methods, J. Process Control 24 (2014) 1156–1178, http://dx.doi.org/10.1016/j.jprocont.2014.03.010.

[6] M. Ellis, P.D. Christofides, Real-time economic model predictive control of nonlinear process systems, AIChE J. 61 (2015) 555–571, http://dx.doi.org/10.1002/aic.14673.

[7] C. de Prada, J.L. Pitarch, Real-time optimization (RTO) systems, in: Resource Efficiency of Processing Plants, Wiley Online Books, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2018, pp. 265–292, http://dx.doi.org/10.1002/9783527804153.ch11.

[8] S. Engell, Feedback control for optimal process operation, J. Process Control 17 (2007) 203–219, http://dx.doi.org/10.1016/j.jprocont.2006.10.011.

[9] E.M. Gómez Sayalero, A Study on Modelling, Data Reconciliation and Optimal Operation of Hydrogen Networks in Oil Refineries, Universidad de Valladolid, 2016, http://dx.doi.org/10.35376/10324/16637.

[10] OPAF, Open process automation^{TM} forum [WWW Document], 2018, https://www.opengroup.org/forum/open-process-automation-forum (accessed 6.1.20).

[11] C.R. Cutler, L.B. Ramaker, Dynamic matrix control— a computer control algorithm, in: AIChE 86th Spring Meeting, Houston, Texas, 1979, Paper No. 51b.

[12] C. de Prada, D. Sarabia, E. Gutierrez, S. Marmol, M. Sola, C. Pascual, R. Gonzalez, Integration of RTO and MPC in the hydrogen network of a petrol refinery, Processes 5 (2017) 3, http://dx.doi.org/10.3390/pr5010003.

[13] A. Galan, C. de Prada, G. Gutierrez, D. Sarabia, I.E. Grossmann, R. Gonzalez, Implementation of RTO in a large hydrogen network considering uncertainty, Optim. Eng. (2019b) http://dx.doi.org/10.1007/s11081-019-09444-3.

[14] S. Skogestad, Plantwide control: the search for the self-optimizing control structure, J. Process Control 10 (2000) 487–507, http://dx.doi.org/10.1016/S0959-1524(00)00023-8.

[15] D. Sarabia, C. de Prada, E. Gómez, G. Gutierrez, S. Cristea, J.M. Sola, R. Gonzalez, Data reconciliation and optimal management of hydrogen networks in a petrol refinery, Control Eng. Pract. 20 (2012) 343–354, http://dx.doi.org/10.1016/j.conengprac.2011.06.009.

[16] A. Galan, C. de Prada, G. Gutierrez, D. Sarabia, R. Gonzalez, M. Sola, S. Marmol, Validation of a hydrogen network RTO application for decision support of refinery operators, IFAC-PapersOnLine 51 (2018) 73–78, http://dx.doi.org/10.1016/j.ifacol.2018.09.256.

[17] EA Internacional, PROOSIS, 2019.

[18] A. Alessandri, M. Baglietto, G. Battistelli, V. Zavala, Advances in moving horizon estimation for nonlinear systems, Proc. IEEE Conf. Decis. Control (2010) 5681–5688, http://dx.doi.org/10.1109/CDC.2010.5718126.

[19] J.B. Rawlings, State estimation using moving horizon estimation and particle filtering, UW Math. Probab. Semin. (2009) 1–45.

[20] J.B. Rawlings, L. Ji, Optimization-based state estimation: Current status and some new results, J. Process Control 22 (2012) 1439–1444, http://dx.doi.org/10.1016/j.jprocont.2012.03.001.

[21] V.M. Zavala, C.D. Laird, L.T. Biegler, A fast moving horizon estimation algorithm based on nonlinear programming sensitivity, J. Process Control 18 (2008) 876–884, http://dx.doi.org/10.1016/j.jprocont.2008.06.003.

[22] J.D. Hedengren, A.N. Eaton, Overview of estimation methods for industrial dynamic systems, Optim. Eng. 18 (2017) 155–178, http://dx.doi.org/10.1007/s11081-015-9295-9.

[23] C.V. Rao, J.B. Rawlings, in: F. Allgöwer, A. Zheng (Eds.), Nonlinear Moving Horizon State Estimation BT - Nonlinear Model Predictive Control, Birkhäuser Basel, Basel, 2000, pp. 45–69.

[24] N. Arora, L.T. Biegler, Redescending estimators for data reconciliation and parameter estimation, Comput. Chem. Eng 25 (2001) 1585–1599, http://dx.doi.org/10.1016/S0098-1354(01)00721-9.

[25] B. Nicholson, R. López-Negrete, L.T. Biegler, On-line state estimation of nonlinear dynamic systems with gross errors, Comput. Chem. Eng 70 (2014) 149–159, http://dx.doi.org/10.1016/j.compchemeng.2013.11.018.

[26] A. Galan, C. De Prada, G. Gutierrez, D. Sarabia, R. Gonzalez, Predictive Simulation Applied To Refinery Hydrogen Networks for Operators' Decision Support, IFAC-PapersOnLine 52 (2019a) 862–867.

[27] L.T. Biegler, Nonlinear Programming, Society for Industrial and Applied Mathematics, Society for Industrial and Applied Mathematics, 2010, http://dx.doi.org/10.1137/1.9780898719383.

[28] Y. Cao, S. Li, L. Petzold, R. Serban, Adjoint sensitivity analysis for differential-algebraic equations: The adjoint DAE system and its numerical solution, SIAM J. Sci. Comput 24 (2003) 1076–1089, http://dx.doi.org/10.1137/s1064827501380630.

[29] Y. Cao, S. Li, L. Petzold, Adjoint sensitivity analysis for differential–algebraic equations: Algorithms and software, J. Comput. Appl. Math 149 (2002) 171–191, http://dx.doi.org/10.1016/S0377-0427(02)00528-9.

[30] R. Serban, C. Petra, A.C. Hindmarsh, User documentation for idas v3.1.0 (sundials v4.1.0) [WWW Document], 2019, https://computation.llnl.gov/sites/default/files/public/idas_guide.pdf (accessed 6.18.19).

[31] P. Gill, W. Murray, M. Saunders, SNOPT: An SQP algorithm for large-scale constrained optimization, SIAM Rev. 47 (2005) 99–131, http://dx.doi.org/10.1137/S0036144504446096.

[32] P.E. Gill, W. Murray, M.A. Saunders, E. Wong, User'S Guide for {SNOPT 7.7}: Software for Large-Scale Nonlinear Programming, La Jolla, CA, 2018.