Predictive Simulation Applied to Refinery Hydrogen Networks for Operators' Decision Support

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Abstract: Hydrogen networks are essential in modern oil refineries for they supply the main reactant for hydrodesulphurisation processes. These networks are usually integrated in a complex fashion, and sensitive to changes in any of their process units. In addition, plant measurements and prediction tools available, tend to be insufficient to make educated decisions when unexpected changes realize, especially on-line. This study presents an embedded dynamic estimator within a simulation framework, which uses plant data to estimate states and parameters of a hydrogen network and predicts its future behavior. A representative process network of three consumers and two sources is the case study utilised to demonstrate the usefulness in their decision-making process of operators. For this purpose, a brief what-if-analysis is discussed. In the last section, future challenges and directions of this predictive simulation tool are highlighted.

Keywords: MHE, parameter estimation, process simulation, what-if-analysis.

1. INTRODUCTION

1.1 Context

Environmental impact and process efficiency have driven process automation and optimisation deployment across the process industry. In particular, industry seeks minimisation of equipment's downtime and off-spec production, while keeping process safety. Hence, automatic control, simulation and optimisation tools are gaining relevance and set-up new challenges for these techniques to aid process operators at all levels.

In this context, how to properly deal with uncertainty becomes crucial since it may have an impact not only in product specifications, but also in process safety and assets' integrity as well. Therefore, research and development of decision support tools is essential to better aid operators in their decision-making process, especially under uncertain conditions.

Naturally, effective simulation techniques that accurately predict future states and variables of the process, given some scenario conditions, would draw interest from operators. Moreover, if the simulation initiates at current process conditions, then it is called predictive simulation (PS). For better illustration of the concept we focus on a particular process example (i.e.: hydrogen networks) to develop and explain PS usefulness for operators.

1.2 Hydrogen networks

For instance, hydrogen (H₂) is mostly consumed in oil refineries in hydrodesulphurisation (HDS) units as reactant for sulphur removal of distilled and cracked streams. This is how refineries meet fuel sulphur content specifications that redound in less pollution from fuels consumption. In addition, some H₂ is consumed in hydrocracking (HDC) units that basically break down long chain hydrocarbon (HC) molecules from vacuum distillation, and produce lighter HC cuts that are more valuable.

Typically, H₂ is distributed through a complex network system, which is supplied by H₂ producers (e.g.: steam reformers and platformers) and feeds consumer units. Each consumer is either an HDS or HDC unit with its own process requirements, especially regarding H₂ purity in the recycle and treatment gas stream. That is why networks comprise several distribution headers, usually associated to different H₂ purities, namely: high (HPH), low (LPH) and fuel (FGH). HPH contains H₂ purities over 90% and is fed by steam reformers. LPH contains over 70% H₂ purity and is fed by platformers and recycle purge from consumers. FGH collects gases with less than 70% H₂ content, typically excess gases from LPH and consumers (De Prada et al, 2017; Gomez, 2016). Only HPH and LPH gases could be used as make-up (MU) gas to the consumer units. Figure 1 presents a generic schematic of a H₂ network at the top and a scheme of an actual network at the bottom (Gomez, 2016).

In this study we present a PS formulation, which embeds dynamic state estimation in a simulation environment. The
structure of the paper starts with the problem statement in section 2, introducing the explicit objectives. Then we present the dynamic model used in the case study in section 3. Section 4 discusses the dynamic state estimation technique and how embeds in the simulation environment. Section 5 focuses on the predictive simulation description and the case study results. Lastly, in section 6 we present the conclusions and future directions of predictive simulation and its usefulness for decision support.

Fig. 1. Top: generic H₂ network schematic with sources (HS1/2), consumers, high purity headers (HPH 1/2), low purity header (LPH), and fuel gas header (FGH). Bottom: Petronor, Somorrostro refinery H₂ network in Muskiz, Spain (Gomez, 2016).

2. PROBLEM STATEMENT

Firstly, we address a dynamic state estimation problem with the following statement.

Given:

- a H₂ network dynamic model (DM),
- plant measurements of gas and HC flowrates, and H₂ purity (i.e.: plant data),
- previous manipulated variables' (MVs) values

Estimate current state variables such that DM variables and plant data difference is minimised along a past rolling horizon of N sample times. Namely, solve the so called: moving horizon estimation (MHE), for the H₂ network (Alessandri et al, 2010).

Equations (1-8) show the mathematic formulation of the MHE problem, given a continuous-time dynamic system.

\( f(x(t), \dot{x}(t), u(t), p, w(t)) = 0, \quad x(0) = z_0. \)  
\( y(t) = h(x(t), u(t), p, v(t)). \)  

Where \( z \) represents the state vector, \( u \) the control vector and \( w \) the additive disturbance of the system, \( \dot{z} \) is the derivative of \( z \), and \( p \) the vector of parameters (1). State vector is observed through measurements \( y \), and \( v \) is the measurements noise vector (2). We aim to determine estimates of current states given past information over a "sliding time window" \([t-N, t]\), then \( \hat{z}(\cdot) \), represents the information vector collected (3). State estimates are represented by \( \hat{z} \).

Therefore, the minimisation problem of the state estimation could be expressed as per (5-8).

\[
\min \left\{ \left\| \hat{x}_{k-N} - z_{k-N} \right\| \right\} + \sum_{k=N}^{t} \left\| \Delta w_{k} \right\|^2 + \sum_{k=0}^{t} \left\| y_{k} - y_{k}(\cdot) \right\|^2 \right\}
\]

Such that:

\( \hat{z}_0 \leq \hat{z}_k \leq z_{n_k} \quad k = 0, \ldots, N \)  
\( y_0 \leq y_m \leq y_{n_k} \quad k = 0, \ldots, N \)  
\( \Delta w_0 \leq \Delta w_k \leq \Delta w_{n_k} \quad k = 0, \ldots, N \)

Where: \( R, Q \) and \( P \) are positive definite matrices that weight each term of the cost function. The first term, represents the quadratic arrival cost (Alessandri et al, 2010; Zavala and Biegler, 2009), being "\( \bar{z} \) bar" the previous estimation of \( \hat{z} \). The second term, accounts for the states' evolution of \( \hat{z} \) considering (1). The third term, accounts for the distance between actual measurements and estimations (2).

Secondly, we run a simulation to assess future states of the network under different meaningful scenarios. Basically integrating over time, in this case \([t, t_{\text{final}}]\), applying \( \hat{z} \) as initial state vector.

In overall, this MHE embedded in a simulation framework becomes a PS.

3. DYNAMIC MODEL

3.1 H₂ consumers

A first principle model is used to represent all consumer plants and headers. In particular, H₂ consumption in reactors is simplified to first order kinetic in terms of HC loads, since H₂ is required in great excess to protect catalysts premature deactivation. A schematic of plant HDS1 is shown in Fig. 2 for ease of understanding of the model. Here we present only the most relevant equations, while a complete explanation of the dynamic model is available for consultation in previous works of Galan et al (2017) and Gomez (2016).

The model considers two mechanisms of H₂ consumption: chemical reaction (in reactors) and solubility losses (in separators). Additionally, reactors and separators both have a lagged response due to their volume (hydraulic residence time). In short, dynamics of consumer units are simplified as
first order ones to account for residence time in reactors and separators (Galan et al, 2017).

In terms of chemical components the model considers: H$_2$, light compounds (LIG) that represent aggregated hydrocarbon fractions cracked in the reactors, and HC. These components compose process streams. A colour code identifies stream's nature: being: green (liquid-gas mixture), orange (liquid), and blue (gas). For instance, in Fig. 2 the flow diagram of HDS1 is shown, including instrument tags and streams colour code.

Equations (9-10) represent H$_2$ consumption ($H_2$CON), and LIG generation ($LIG_{GEN}$) in reactors as function of HC feed ($HC_{IN}$).

\[
H_2\text{CON} = k_{H_2HC} \times HC_{IN} \quad (9)
\]

\[
LIG_{GEN} = k_{LIGHC} \times HC_{IN} \quad (10)
\]

Separation drums (SHP/SMP) have specific additional equations (11-12), fully described by Gomez (2016), that represent how they split their mixed gas and liquid inlet ($G_{IN}$) streams into a gas outlet ($F_{OUT}$) and mixed gas and liquid outlet ($G_{OUT}$). The latter containing the gases that remain solubilised from the $G_{IN}$. A solubility constant for: gas in HC and H$_2$ in HC, should be considered for this behaviour to be useful (Galan et al, 2017; Gomez, 2016; Sarabia et al, 2012). In the particular case of LP drums $G_{OUT}$ is free of gases (Galan et al, 2017).

\[
G_{as} = k_{GHC} \times HC_{IN} \quad (11)
\]

\[
G_{OUT} \times y[H_2OUT] = k_{H_2HC} \times HC_{IN} \quad (12)
\]

Where $k_{GHC}$ and $k_{H_2HC}$ are the solubilities of gas and H$_2$ in HC respectively, $HC_{IN}$ is the HC inlet to the drum.

4. MHE EMBEDDED IN SIMULATION

We developed an automatic calculation procedure capable of running a dynamic simulation based on the states estimations from an embedded MHE.

4.1 Procedure description

The calculation starts once actual measurements are available (step 1) and ends the last simulation is run to predict future states (step 9). In Fig. 3 a diagram of the main steps of the procedure are shown.

Steps 1-3 are required to run the optimisation, and basically get information from the process and perform some standard calculations at each sample time.

Steps 4-4’ refer to the optimisation itself to obtain the states estimations. In this case we applied a sequential approach, thus we can take advantage of the simulation environment and reduce significantly the number of decision variables passed to the optimisation engine. Instead of simultaneously solving the optimisation for all variables, this method iterates the optimiser results and model integration on the explicit variables from the simulation.

Steps 3-6 perform the actual state estimation (*SE, Fig 3), which the continuous simulation is run to predict future states.

4.2 Implementation

It is implemented on PROOSIS® (2018) and the optimisation engine is SNOPT (Gill et al, 2008; Gill et al, 2005).

Based on the procedure presented in Fig. 3, and considering the specifics of PROOSIS® (2018) environment, we developed the actual tool to apply on to the case study. The main characteristics are shown in Fig. 4. Namely, the model itself is coded in a component, and classes enable the integration of external programs (not coded on PROOSIS) such as SNOPT engine from the same environment. Finally, the simulation is actually run through an experiment (executable module in PROOSIS®) from where the user can set up the integration time, boundaries and control variables.
5. PREDICTIVE SIMULATION

In order to understand how this PS could be used for decision support of operators, we implemented it on to a case study of a H₂ network. This case study is inspired in the actual H₂ network model of Petronor, but rather simplified to better test this prototype PS tool. Details of the actual Petronor process network are presented by De Prada et al (2017) and Sarabia et al (2012).

5.1 Case study

We set up a theoretical H₂ network, which comprises three consumer units, namely HDS1/2/3, and two H₂ sources, namely HS1/2. Gas is distributed throughout the network from one HPH, supplied by HS1/2, and a LPH. See Fig. 5 for more details on the network topology. HDS2/3 internal topology is presented in Fig. 6 (top for HDS2, and bottom HDS3). HDS1 schematic is shown in Fig. 1.

A summary of statistics of the network model is presented in Table 1. PS is run on a PC Intel® Core™ i7-6500U CPU @ 2.50 GHz RAM 16 GB, and takes on average 40s per sample time to complete the execution.

It is clear that in all three units, estimations improve over time, being more accurate for HDS2/3, and less for HDS1. In addition, HDS1 is more sensitive to recycle gas purity system (Galan et al, 2017). In Fig. 7, measured and estimated recycled gas purities for each unit are presented in a scenario where H₂ purity is deficient in HDS1.
changes than HDS2/3, since it dropped almost 20% purity (from 60% to 40%) when the rest lost half of that at the sample time (see Fig. 7). This information could be critical in order for operators to take action quicker in HDS1, rather than give equal priority to all the units in the event of an upset.

Fig. 7. Recycle gas purities in HDS1/2/3. Top: actual continuous. Bottom: measured (full line) and estimated (dash line). H<sub>2</sub> purity lower limit (dotted line).

5.2 What-if-analysis

As a brief example of what-if-analysis (WiA) we present alternative scenarios that could correct a very low H<sub>2</sub> purity in recycle gas in HDS1, such as the one shown in Fig. 7 (scenario 01).

For instance, it is possible to increase purity in HDS1 by increasing recycle purge (MV4), reducing HC load (MV1) and reducing MU gas from LPH (MV2). If we try these changes, gas purity changes drastically (Fig. 8 top, scenario 1A). However, operators will usually be reluctant to decrease load due to the economic impact in the process benefits. Therefore, another alternative could be cutting back MV2, which should allow more room for high purity H<sub>2</sub> in the make-up while keeping recycle purge high and unit feed. Still some H<sub>2</sub> could be saved by reducing high purity make-up in HDS2 (MV1), being this an option more cost-effective than the former (Fig. 8 bottom, scenario 1B).

Another scenario of interest is when unexpected malfunctions occur to critical equipment. For instance, a feed pump of HDS2 trips due to a short circuit in its power motor. As a consequence, HDS2 losses 30 m<sup>3</sup>/h (15%) of feed at sample time 1, and recycle gas purity increases abruptly (see Fig. 9 top).

Under these circumstances, operators should try to process the remaining load of HDS2, however only 10 m<sup>3</sup>/h can be taken by HDS1 and nothing by HDS3. Therefore, efforts may be given to minimise H<sub>2</sub> excess. An intuitive alternative is to decrease high purity MU gas in HDS2, and increase low purity MU in HDS1. The result of this strategy is shown in Fig. 9 (bottom).

Fig. 8. Alternatives to increase recycle gas purity in HDS1, scenarios 1A/B. Top: increase purge (MV4), reduce load and LPH make-up gas (MV1 and 2, respectively).

An interesting concept of WiA is that it may be more intuitive to carry out by non-expert users, such as operators, due to the fact that it simply assumes conditions of the system. Control room operators should be capable of setting up realistic scenarios for analysis, regardless of their modelling and programming skills. For instance, an operator could quickly familiarise with the variables and may even test by himself several alternatives. That is not usually the case of optimisation tools, such as real-time optimisers (RTO) or model-predictive controllers (MPC). Furthermore, in this point PS has an advantage over other decision-making approaches, due to its intuitiveness. Hence, it might be easier to deploy in an industrial facility than other tools. Conversely, an RTO and MPC seek optimal solutions, rather than trying a reduced set of alternatives as in the case of WiA (we assume that operators can test just a few scenarios). That is why in this aspect an optimisation approach is advantageous over a PS tool. Bearing these features in mind,
it may be wise to combine them. For instance, given an RTO solution, an operator may check how the process dynamics respond to set point changes, at the time that the RTO already took care of optimising the new steady state. Likewise, an MPC may not capture some insights of equipment transient restrictions, which an operator could be aware of, and therefore replicate the main variables directions but previously checked on the PS tool. Some of these ideas were also presented by Galan et al (2018).

One important aspect to explore in future studies could be PS as a support tool for steady state optimisation, such as RTO. In fact, it may allow operators to assess different alternatives to reach new steady states due to the incorporation of dynamic models from the PS. Another direction of research might be to embed MPC as well, and therefore the tool could have MHE, optional PS or MPC, depending on the situation. In any case, it would provide a set of options to support operators in their decision-making process.

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REFERENCES

Alessandri, A., Baglietto, M., Battistelli, G., Zavala, V. (2010). Advances in moving horizon estimation for nonlinear systems, 49th IEEE Conference on Decision and Control (CDC), Atlanta, GA, pp. 5681-5688. doi: 10.1109/CDC.2010.5718126

De Prada, C., Sarabia, D., Gutierrez, G., Gomez , E., Marmol, S., Sola, M., Pascual, C., Gonzalez, R. (2017). Integration of RTO and MPC in the Hydrogen Network of a Petrol Refinery, Processes, 5, 3, ISSN 2227-9717.

Galan, A., De Prada, C., Gutierrez, G., Sarabia, D., Gonzalez, R., Sola, M., Marmol, S. (2018). Validation of a hydrogen network RTO application for decision support of refinery operators, in: Zenodo. doi:10.5281/zenodo.1405654

Galan, A., De Prada, C., Gutierrez, G., Gonzalez, R. (2017). Dynamic simulation applied to refinery hydrogen networks, in: Zenodo. doi:10.5281/zenodo.1013258

Gill, P. E., Murray, W., Saunders, M. A. (2008). SNOPT 7 User's Guide.

Gill, P. E., Murray, W., Saunders, M. A. (2005). SNOPT: An SQP algorithm for large-scale constrained optimization, SIAM Review, 47(1), pp. 99-131.

Gomez, E., (2016). A study on modelling, data reconciliation, and optimal operation of hydrogen networks in oil refineries, Doctoral thesis, University of Valladolid, Spain

PROOSIS®, (2018). Propulsion object-oriented simulation software. Empresarios Agrupados Internacional.

Sarabia, D., de Prada, C., Gomez, E., Gutierrez, G., Cristea, S., Sola, J., Gonzalez, R. (2012). Data reconciliation and optimal management of hydrogen networks in a petrol refinery, Control Engineering Practice, Volume 20, Issue 4, pp 343-354, ISSN 0967-0661, https://doi.org/10.1016/j.conengprac.2011.06.009.

Zavala, V.M., Biegler, L.T. (2009). The advanced-step NMPC controller: Optimality, stability and robustness, Automatica, Volume 45, Issue 1, pp. 86-93, ISSN 0005-1098, https://doi.org/10.1016/j.automatica.2008.06.011.